

# **Systems Analysis of Stock Buffering**

Development of a Dynamic Substance Flow-Stock Model for the Identification and  
Estimation of Future Resources, Waste Streams and Emissions

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Systems Analysis of Stock Buffering: Development of a Dynamic Substance Flow-Stock Model for the Identification and Estimation of Future Resources, Waste Streams and Emissions

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*To my parents*



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## **Chapter 1    Introduction**

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## 1.1 Introduction

Over the last century, the increase in the global population and the growth of the economic activities have been accompanied by an increase in demand for materials, with a consequent increase in extracting, processing, using and waste treatment activities. These economic activities give rise to environmental problems. Some of these problems are related to the extraction of resources, others to emissions and waste flows resulting during the life cycle of these materials including energy resources.

A number of analytical tools have been developed to manage the environmental impact of extraction and emission related problems. These include Life Cycle Assessment (LCA), Material Flow Analysis (MFA), Substance Flow Analysis (SFA) and physical Input / Output (I/O), which in different ways study the flows of substances, materials and products through the economic system and their impacts on the environment. Each of these tools has its own purpose and methodology (see Heijings, 1997, van der Voet, 1996, Fisher-Kowalski, 1998). LCA is a tool for analysing the environmental burden of a product through all the stages in its life cycle, from the extraction of resources, through the production of materials, product parts, the product itself and its use, to its management after it is discarded, either by reuse, recycling, or final disposal (Guinee et al., 2001). MFA is an analytical tool that systematically describes material flows, generally for a region, expressed in physical units (kilograms, tons), through extraction, production, transformation, use, recycling, and final disposal as waste or emissions. MFA has been used to evaluate losses during the material life cycle and to provide measures for the more efficient use of resources (Bringezu, et al., 1997). MFA can be performed on different levels. It is performed to include the total material flows within the system, which is referred to as bulk MFA (Kleijn, 2001) or for specific materials such as biomass, or in a narrower sense for a chemical element or compound, which is referred to as SFA.

SFA is an analytical tool that is used to describe or analyze the flows of one or more substances into through and out of a system. It has been used to identify the direct, economic and ultimate causes of environmental problems (for example for Cadmium soil load, the direct cause is atmospheric deposition, which is caused by incineration. Its ultimate origin lies in the flow of zinc) and to identify the most effective policy measures to eliminate or to reduce them (van der Voet, 1996).

Within the framework of SFA, several types of analysis can be used. These include accounting and static and dynamic modelling. So far the attention in the SFA community has been focused mainly on drawing accounts and on comparative static modelling (Bringezu et al., 1997; Bauer et al., 1997; Anderberg et al., 1995). Recently it has been acknowledged that an important difference between static and dynamic models lies in the inclusion of stocks in society: substances accumulated in the stocks of materials and products in households or in the built environment (Bergbäck & Lohm, 1997; Fraanje & Verkuiljen, 1996). These stocks can be very large and, sooner or later these will lead to waste and emissions. The present stock of materials in society will strongly influence future waste streams and emissions of many hazardous substances to the environment.

Matthews et al. (2000) have shown that the growth of such stocks is not restricted to individual or isolated substances or materials, but overall is a significant phenomenon in society. The total societal stock (of materials) increases each year by approximately one third of the total yearly material inflow. Most of this goes into materials for building and other infrastructure. At some point in the future demolition waste streams can be expected to rise.

Other studies have shown a decline in point source emissions within most industrialized countries. However, future emissions from built-up stocks may be considerable. Bergbäck and Lohm (1997) and Guinée et al., (1999) have argued that emissions of heavy metals have decreased over the past decades, but at the expense of a stock increase. This includes not only the stock that is in use, but also materials that have been kept in storage or left underground. Bergbäck and Lohm (1997) concluded that such “hibernating stocks” might be very large. Kleijn and van der Voet (1998) pointed out that the future worldwide emissions of CFCs from present stocks would be in the same order of magnitude as accumulated past emissions, even assuming a complete phase-out of this chemical.

A crucial issue for environmental policy, therefore is to forecast future emissions in order to anticipate future problems and take timely action. However, models used for estimating future emissions and waste

streams mostly ignore the stocks, due to a lack of data and insufficient insight in the dynamics of such stocks. In consequence they are completely left out of environmental forecasts.

Economic models are often used to estimate future emissions. They are used to explore future production and estimate future emissions by assigning emission factors to this production. For waste, a generally similar approach is used: the volume of waste streams is assumed to be directly related to economic development. While this approach has some value on a general level, it clearly leads to dubious outcomes when looking at emissions of specific substances and waste streams of specific materials. Economic models usually ignore some of the crucial mechanisms that underlie the generation of waste and emissions (van der Voet and Kleijn, 2000). They particularly ignore physical laws, such as mass balance and stock building over time. Such shortcomings in economic analysis have been discussed in several studies (Georgescu-Roegen 1973, Ayres, 1997, Heijungs, 1997). Another way to predict future emissions is to use material flow models. These models capture some aspects much better, but are limited to physical considerations and do not include costs or description of the mechanisms of economic analysis. These models have no rationale for predicting any future developments, other than applying mass balance. To obtain more accurate predictions, elements from both types of models should be combined. Recently several studies have pointed out the need to combine physical models with economic models (Boumann et al., 2000, Brunner, 2002 and Kytzia and Nathani, 2004) and some attempts have been made to integrate these two approaches (Ayres and Kneese, 1969, Leontief, 1970, Victor, 1972, Ruth, 1993 and Feber and Proops, 1997, Elshkaki et al., 2002).

This chapter provides an introduction to the thesis. The following section describes the aim and scope of the research presented in this thesis, section 3 contains the scientific background, section 4 discusses the main issues addressed in this thesis, section 5 describes the selected case studies and section 6 outlines the structure of this thesis.

## **1.2 Aim and scope**

The first main aim of this thesis is to systematically gain insights into the mechanisms that determine the generation of future emissions and waste flows from present stocks due to both socio-economic and physical/chemical aspects. It seeks to find ways to integrate these insights into substance flow models that can explore future emissions and resource availability in a meaningful manner. It then employs this model, using stock dynamics and combining elements from both economic and physical models, to evaluate the effectiveness of different policy options.

As such, the research presented in this thesis follows three consecutive stages:

- The first part develops a dynamic stock model, which combines elements from both physical and economic models, in order to estimate current and future waste streams, emissions and resources, and establish a link to a flow model, thus creating a dynamic substance flow-stock model (chapter 3 of this thesis).
- The second part develops a software tool able to carry out such a model.
- The third part implements the model in two case studies relevant to environmental policy (chapters 4 to 8 of this thesis). The first case study investigates the environmental and economic consequences of the development of lead stocks in the EU (chapter 4) and The Netherlands (chapters 5 to 7). The second case study investigates the potential impacts of using platinum in the newly introduced Fuel Cell technology and addresses issues of both resource availability and environmental impacts (chapter 8).

## **1.3 Scientific background**

Substance flow analysis (SFA) originates from natural and engineering sciences (van der Voet, 1996; Ayres, 1998) and falls within a relatively new scientific field of research: Industrial Ecology. Industrial

Ecology, also called the science of sustainability, is formulated in a way that is analogous with ecology. It is concerned with studying society's metabolism to analyze the causes of environmental problems and indicate possibilities for more sustainable management of materials (Graedel and Allenby, 1995).

SFA considers the physical dimension of the economy as described in the concept of industrial metabolism (Ayres, 1989). This term is defined as the set of physical and chemical transformations that convert raw materials (biomass fuels, minerals, metals) into manufactured products and structures ("goods") and wastes (Ayres and Simonis, 1994). SFA focuses on the industrial metabolism of substances. It determines their main entrance routes to the system, transformation or storage within the system and output from the system.

SFA is one of the main analytical tools within the research field of industrial ecology, which is largely driven by engineering approaches and systems perspectives (Ruth, 2006). It is used to describe or analyze the flows of one substance or group of substances in, through and out of a system (van der Voet, 1996). SFA considers physical entities, often a geographical area, and is divided into two subsystems: the economic or societal and the environmental. Systems analysis is the science dealing with complex systems and interactions within those systems. It does so by applying mathematical methodologies to form an overall picture of the systems. Two types of system analysis methods can be distinguished; hard and soft systems analysis (Checkland, 1981). Hard system analysis is a scientific approach for problem solving, which deals with well-defined problems and which aims to provide an ideal and unambiguous solution. Soft system analysis is a qualitative technique, which deals with poorly defined problems with a possibility of different interpretations. Its outcome is more generally improved understanding, rather than a specific solution. SFA is a hard system analysis approach.

The system flows and stocks in SFA are quantified either by accounting or by modelling (substance flow accounts, static SFA models, and dynamic SFA models). The dynamic SFA model includes stocks in society, and combines physical, socio-economic and engineering elements. Stocks of products and materials in use represent a major reservoir of materials that cause a disconnection between the inflows and outflows through the economic subsystem in any one year. This is because substances, locked into applications with a long life span, such as building materials or durable user goods, have a long residence time in society. The dynamics of the growth and decline of the stocks of any substance over time are determined by the inflow and outflow of materials and products that contain it. The inflow is determined by the demand for the products containing those materials and substances, and can be derived from socio-economic information. The outflow is mainly determined by two physical mechanisms, those of leaching and delay. The delayed outflow is based on residence time theory, well-established theory in chemical engineering (Melo, 1999).

The results of SFA are interpreted by transforming the overview of the system flows and stocks into policy relevant information that uses specific indicators (Van der Voet, 1999, 2000) and/or Life Cycle Analysis (LCA) impact categories (Tukker, 1996; Udo de Haes et al., 1999), which are based on environmental science. SFA can further be used as input for further analysis mainly risk assessment.

## **1.4 Issues addressed in the thesis**

Resource availability and environmental quality start to become serious problems when the extraction of resources, the emissions of hazardous substances and the disposal of waste occur at rates that exceed the capacity of the natural system (Braat and Lierop, 1987). Issues and concepts related to the world's finite resources and limits for expansion, the principals of the conservation of mass and the constraints imposed by the first and second laws of thermodynamic on the effective use of resources have been widely discussed (Meadows et al., 1972, Rothmans, 1990, Alcamo et al., 1993, Ayres, 1999, Tilton, 1999, and Tilton, 1996).

In this thesis, the main issues discussed relate to the availability of resources, especially those required for new technologies that aim to increase sustainability, the emission of hazardous substances and to waste flows.

### 1.4.1 Resource problems

Resource problems, which can occur with both renewable resources (such as fish, timber and topsoil), or non-renewable ones (such as minerals and fuels) occur when there is shortage of supply of resources required for production and consumption.

The depletion of resources was predicted several decades ago by the Club of Rome in their publication “Limits to Growth” (Meadows et al., 1972), which was based on a system dynamic model. Since the publication of their report, interest in the issue of resource depletion has declined somewhat, particularly over the availability of ores. This is mainly due to the observation that the world is not running out of mineral resources, as the profitable extractable reserves of many commodities has in fact increased. Recent concern about the depletion of resources has shifted towards the question of the depletion of renewable resources, such as rainforests and fish stocks. However, the discussion about the availability of mineral resources is still ongoing. Tilton (1996) points out that the debate not only continues but has become even more polarized with two schools holding two different views. The first school, often made up of ecologists and engineers, is concerned about the limitations of the earth in supporting current and anticipated demand for exhaustible resources. The second school, often composed of economists, claims that with the help of market incentives, public policies and new technology the earth can meet society’s needs for an indefinite future.

The latter group cite evidence that cost reductions due to the new technology will make more resources available and that these will exceed cost increases caused by the depletion of cheaper deposits (Reynolds, 1999). Equally, before resources are exhausted, demand will decline due to rises in the cost, simultaneously stimulating the development of alternatives and increasing the stock (Hotelling, 1931). The first school argues that increases in profitable extractable reserves are due to the availability of cheap energy sources from fossil fuels that are being rapidly depleted (Richards, 2006) and whose use creates serious and long-term environmental impacts. This shift in the problem was predicted by the authors of the limits to growth when they revisited the issue in their subsequent book “Beyond the Limits” (Meadows et al., 1992), in which they predicted a collapse of modern civilization due to the environmental damage caused by the over-production and over-consumption of resources.

### 1.4.2 Emissions and waste problems

Emissions and disposal of waste and by-products from economic activities and the associated energy used in these activities can give rise to changes in environment quality. These problems involve both macro and micro-pollutants. Problems related to macro-pollutants include the overload of specific substances in specific environmental mediums. Examples include, global warming which is caused by the increase in the stock of CO<sub>2</sub> in the atmosphere and eutrophication, which is caused by the increase of nutrient stocks in lakes and shallow coastal waters. Problems related to micro-pollutants include the emission of certain noxious substances, even in small quantities, which disturb natural processes and threaten the health of humans and ecosystems due to their toxicity, carcinogenicity, mutagenicity or hormone mimicking properties. Examples include persistent organic micro-pollutants and heavy metals, both of which are generally emitted in small quantities but accumulate in the environment because of their non-degradability (Van der Voet et al., 2000).

Several measures can be taken to address these problems. These include end-of-pipe technologies, increasing recycling and phasing out hazardous intended or non-intended applications. Some argue that advances in technology can provide a solution to most of these problems. For example several remedial technologies (physical, chemical and biological) have been introduced to address problems of emissions and waste. It is argued that physical treatment technologies, such as landfill or dilution and dispersal through smokestacks do not provide effective solutions due to the limits imposed by the principals of the conservation of mass. Thus these technologies transfer risk from one place to another or from the present to the future. Chemical and biological treatment technologies, while often more effective than physical technologies, can also have undesirable side-effects (Huesemann, 2001).

Recently industrial ecologists have been reinforcing and underpinning earlier arguments about the possibility of preventing environmental pollution by redesigning industrial processes (i.e. industrial processes with zero emissions) and closing the material cycle (Ayres and Simonis, 1994; Graedel and Allenby, 1995). While it is possible to substantially reduce emissions, it is not possible to achieve 100% recycling and zero environmental impacts. Industrial processes with zero emissions require significant amounts of energy, which has negative impacts. Moreover, in thermodynamic terms 100% recycling is an impossibility (Huesemann, 2001).

### 1.4.3 Co-production problems

Co-production problems relate to the issues, discussed above, of pollution and resources. In some cases and in the short term, measures aimed at phasing out the use of some substances in some applications appears to be effective. In the longer term however, their effectiveness is questionable, especially in instances involving the co-production of substances. Well-known examples are cadmium recycling (Hupperts et al. 1992) and mercury recycling (Maxson et al., 1991) (see below). Since these substances are co-produced with other materials, increases in demand for the other materials might well lead to an increase in their emissions.

Co-production occurs when the same processes or system produces two or more products. Co-production of products is considered a problem in system modelling within LCA and is normally solved by the technique of co-product allocation (Weidema and Norris, 2002). In terms of substances, co-production is the production of two or more substances from the same process due to the natural existence of substances in the same deposits. In nature, substances exist in the same deposit with different concentration and quantities. Substances with high concentration and large quantities are referred to as host materials and those with low concentration and small quantities are referred to as rare or less abundant materials. The problems of co-production might result from the demand for the host materials or from the demand for rare materials.

Examples of the co-production problems due to the demand for the host materials are those related to the recycling of cadmium and mercury. Cadmium enters the economy as a pollutant in zinc. On the short term, recycling may reduce cadmium emissions, however, on the long term these emissions might increase due to the fact that the inflow of cadmium into the economy is supply driven (i.e. the demand for zinc will increase the supply of zinc and hence of cadmium) (Hupperts et al. 1992). This implies that a reduced demand for cadmium does not result in a reduced supply. A comparable example concerns mercury. The demand for mercury has decreased so much as a result of a strict policy that its supply can be covered completely from by-product sources, such as from the purification of natural gas. An increase in the demand for natural gas will lead to an increase in the supply of mercury. In this case, policies aimed at phasing out or recycling mercury applications therefore might increase its stock in society and consequently an increase in the future emissions (Maxson et al. 1991).

Examples of co-production problems due to the demand for rare metals are those related to the availability of platinum, indium and bismuth. These materials are mostly co-produced with other more abundant materials. Bismuth is mainly found in the same ores with lead, platinum is found with nickel and copper and indium is mainly found with zinc. Some of these rare metals are used in new technologies such as the use of platinum in fuel cell technology or the use of indium in solar cell technology. Others are used to substitute other materials in existing technology such as the substitute of lead by bismuth. For a more widespread use of these technologies, the production of these rare metals must be expanded, especially in the short and medium term when the recyclable stocks in the economy are still being built up. Since their production is linked to that of their "host" materials, this ultimately implies an increased production of these host metals (Zn, Pb, Cu or Ni). Consequently an increased supply of the jointly produced Zn, Pb, Cu or Ni may well have environmental consequences; the more so as lower prices of the host materials will make extraction of the metals from wastes for recycling (here covering all manners of secondary use, including non-intentional secondary applications) less attractive



## 1.5 Case studies

The model presented in this thesis has been applied to two case studies related to heavy metals. Heavy metals cause problems to humans and ecosystems, due to their toxic properties and characteristics. Some of these metals are essential elements however when present in excess, they may create problems of toxicity. Others are not essential and may give rise to toxic manifestations even in small doses (Moolenaar, 1998).

Heavy metals have unique chemical and physical properties, which made them attractive for many industrial applications. Due to their extensive use in the past, especially in applications with long life spans, large stocks of these metals have been built up in the economy. Moreover, they continue to accumulate in the environment due to their non-degradability. Once they have entered the environment they remain there for a long time (Van der Voet et al., 2000). In addition to the direct (intentional) routes, heavy metals can also find their way into the environment, through indirect routes due to for example their presence as contaminants in other resources.

### 1.5.1 The consequences of the development of lead stocks

The first case study deals with lead, which was selected for several reasons. Lead is one of the most extensively used heavy metals in economic processes and consequently, large stocks of lead have been built up in the economy. Environmental concentrations may still be rising due to continuing emissions. Lead also has very toxic characteristics (Scoullou et al. 2001). It is cited by the American Environmental Protection Agency as one of the top 17 chemicals that poses the greatest threat to human beings and the environment (Wu et al., 2004). Lead can cause behavioural problems, learning disabilities, and even death especially among children who inhale or ingest it. In addition lead can be toxic to plants if presents at high concentration, diminishing their productivity or biomass, and eliminating some species (Singh et al., 1997, Xiong, 1997, and Patra et al., 2004).

In the Netherlands there is a policy of reducing lead emissions by phasing out certain lead applications and increasing recycling. The applications from which lead has been phased out include water pipes, paint and gasoline. Since July 2006 an EU directive prevents member states from allowing new electrical and electronic equipments containing lead, mercury, cadmium, chromium VI, and PBB or PBDE to be put on the market (European Commission, 2006). In the short term, the phasing-out policy has resulted in a reduction of lead emissions (Tukker et al. 2001) and recycling has led to less waste containing lead going to landfill. In the long term, however, both measures may have unexpected and undesirable side effects such as an oversupply of lead and a consequent increase in the landfill and incineration streams at the expense of recycling, which may ultimately lead to an increase in emissions. It is argued that for long-term management, more information is required on the dynamic behaviour of substances in the economy (Guinée et al. 1999).

The case study aims to assess the effectiveness of certain policy options and to highlight certain mechanisms that those designing policy need to be aware of. For example, a ban on all applications of a certain heavy metal – the most drastic policy option available – could lead to an environmental problem. These issues are discussed in chapter 5 of this thesis.

In addition to its intentional use, lead is also present in several economic applications, due to its natural occurrence in fossil fuels, other metal and phosphate ores and through secondary flows resulting from the processing of waste flows of its intentional applications. Lead may threat human health through indirect routes of non-intentional flows. For example, lead enters the agricultural chain via phosphate fertilizer and accumulates there, leading to significant concentrations in manure. Processing metal ores and the use of fossil fuels leads to emissions of lead to the environment. Both intentional and non-intentional applications of lead may end up in waste streams. Part of this waste is landfilled, and part is used as fly ash, bottom ash and slag in construction materials. In addition to direct emissions of lead to the air, water and soil, the accumulated lead in roads, buildings, agricultural soil and landfill sites may leach to the soil or ground water.

This case study also aims to evaluate the long-term environmental and economic consequences of the non-intentional flows and stocks of lead and to compare the consequences of these non-intentional flows with those of its intentional flows. An important issue in this case is the one related to resources. The availability of lead in utilized and landfilled secondary materials (fly ash, bottom ash and slag) generated from the production of other heavy metals, electricity production from coal and the incineration of intentional applications of lead provide potential secondary resources for lead. These issues are discussed in chapters 6 and 7 of this thesis.

### **1.5.2 The impacts of using platinum in the newly introduced Fuel Cell technology**

The second case study deals with technologies intended to promote sustainable development. Several new technologies that offer the potential for a transition to a sustainable society require the use of rare often co-produced metals. In the short term, each of these technologies may serve its intended purpose. In the long term, however, there may be side effects that will ultimately limit their combined and wider application. This includes potential bottlenecks in the supply of specific materials and the possible hazards posed by new emissions.

Recent studies have shown that the availability of rare metals may be a real bottleneck in the broad implementation of some new promising technologies (Anderson, 2001 and Graedel, 2002). These metals include indium and germanium (used in solar cell technologies), bismuth and germanium, used in lead-free electronic solder, and some precious metals, i.e. platinum and palladium, used in car catalysts and fuel cells. Active investigation may lead to these limits being overcome, through substitution or through increased availability based on adjoining technological development in primary and secondary production.

This case study aims to systematically determine the resource limitations and emissions problems that the increased use of rare metals in new technologies may give rise to. It does so not for individual technologies, but for a bundle of several such technologies. It also investigates how such resource shortages might be avoided.

These materials are mostly co-produced with other, more abundant, materials such as lead, zinc and nickel. For a more widespread use of these new technologies, production of these rare materials must be expanded, especially in the short and medium term while the recyclable stocks within the economy are being built up. Since their production is linked to that of their "host" materials, this ultimately implies an increased production of these more abundant heavy metals such as Zn, Pb or Ni. This increased supply may well have environmental consequences, the more so as lower prices will make extraction of these metals from wastes for recycling (covering all manners of secondary use, including non-intentional secondary applications) less attractive.

To date the potential impacts of increased demand for co-produced rare metals on the cycles of other metals has not been adequately investigated, either in terms of resource depletion or in the terms of final waste generation and emissions. This case study aims to fill this gap and assess how the potential side effects on the material cycles of the host metals could be limited at an early stage of the technology development. These issues are discussed in chapter 8 of this thesis.

## **1.6 Content of the thesis**

This thesis consists of 9 chapters. Chapters 2 and 3 are dedicated to methodological aspects of substance flow analysis (SFA) and a representation of the dynamic flow-stock model. Chapter 2 includes a general background on substance flow analysis methodology, related modelling aspects and computer tools used in modelling SFA. Chapter 3 describes the substance flow-stock model, the main elements within the system, the relation between flows and stocks and between flows themselves. It quantifies and evaluates these relations, and the factors affecting the dynamic behaviour in the system.

Chapters 4 to 8 include applications of the model in case studies and are based on papers published or submitted to international scientific journals and a chapter in a book. The first case study, concerning the environmental and economic consequences of the development of lead stock-in-use in the EU and Dutch

economic systems, is presented in chapters 4 to 7. Chapter 4 concerns the development of lead stocks in use in the EU. Chapters 5 to 7 explore the same theme in the Dutch context. Chapter 5 describes the modelling aspects, presents the data, and analyzes the long-term management of the intentional use of lead. Chapters 6 and 7 describe the long-term development of the main sources of the non-intentional flows and stocks of lead, evaluate their environmental and economic consequences and compare the consequences of these non-intentional flows to those of intentional flows. The second case study, which concerns the impact of using platinum in the newly developed fuel cell technology in terms of supply constraints and other emissions problems, is presented in chapter 8. Chapter 9 is dedicated to a general discussion, conclusions and recommendations of aspects related to the substance flow-stock model and its applications.

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## **Chapter 2    Substance Flow Analysis – Background and Modelling Aspects**

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## 2.1 Introduction

Modelling is a powerful tool for describing, analysing, operating and evaluating complex systems. It provides an efficient means of communication within the scientific community and between it and policy makers. By definition, models are a simplification of reality and have been defined as ‘a description of the essential aspects of a system, which represent knowledge of that system in a usable form’ (Sinha and Kuszta, 1983). This reflects that models do not include everything, and that this simplification of reality makes models useful (Braat and Lierop, 1987 and Meadows, 2001).

This chapter provides information on modelling in general and substance flow analysis (SFA) models in particular. The following section provides general information on aspects of modelling, section 3 provides information on the SFA framework, section 4 provides a general background on modelling in SFA, which is at the core of this thesis, and section 5 provides general information on computer modelling and software tools used for physical models.

## 2.2 Model types and modelling aspects

### 2.2.1 Model types

Quantitative modelling techniques can be classified according to the purpose they are designed to fulfil. Braat and Lierop (1987) identify four different types:

- descriptive models that are used for to give a general overview of a given problem;
- explanatory models that are based on observation and used to clarify the system;
- predictive models that are used to forecast changes, which include prescriptive, control or management models, that are used for optimization, and;
- evaluative models that are used to assess alternatives.

Descriptive and explanatory models can be an end in themselves or a starting point for developing predictive models, which can either be simulation or prescriptive (optimization) models. Parameter estimates from descriptive models can be used for making predictions (Baron et al., 1990).

Predictive models can be further classified as (Meadows et al., 1974):

- absolute, precise prediction that give exact information about what will happen in the future such as those that predicting natural phenomena;
- conditional, precise prediction that give exact information about what will happen if something else has happened as those for example in process control;
- conditional, imprecise projections of dynamic behaviour that give information about changes in a system if something happens such as those of system dynamic models;
- summary and communication of current trends, relationships or constraints that may influence the future behaviour of a system, and;
- a purely philosophical exploration of the logical consequences of a set of assumptions.

The model developed in this thesis is a predictive model. In SFA, as in other economic and social systems, it is not possible to make precise predictions (in either the absolute or conditional sense) due to uncertainties in the system. In SFA these uncertainties are associated with the estimates of model variables and parameters, which are mainly related to the limited availability and reliability of data and problems of aggregation in the model. Therefore the dynamic SFA model developed in this thesis are time dependent models that can be classified as conditional and imprecise projections of a dynamic behaviour mode.

### 2.2.2 Temporal and spatial

Time and space are important aspects in modelling. In terms of time, models can be static or dynamic, continuous or discrete, deterministic or stochastic. Static systems have a direct and instantaneous link between their variables. Dynamic systems are those in which the variables change without outside influence and their value relies on earlier signals (Ljung and Glad, 1994). Continuous time models are mathematical models that describe the relation between time-continuous signals. They use differential



equations to describe these relationships. Discrete time models describe the relation between sampled signals and use difference equations to describe these relations. Deterministic models work with exact relations (i.e. without uncertainty). Stochastic models are those models that also work with concepts of uncertainty or probability (Ljung and Glad, 1994). In spatial terms models can be global, or cover a specific geographical region. The choice should be based on the nature of the problem at hand: as some problems are local or regional in nature and others are global.

### 2.2.3 Aggregation

The level of aggregation in model design is an important factor in determining the outcome. It may be important in several aspects of the model, such as scale (macro, meso, and micro levels) and time period (second, minute, hour, etc.). Aggregation can also be an issue in terms of the environmental issues at stake (Kandelaars, 1998).

## 2.3 Substance flow analysis

Substance flow analysis (SFA) has been described as a tool to investigate the metabolism of a single substance or group of substances (Udo de Haes, 2000). The current SFA framework was established by Udo de Haes et al. (1997) and contains three elements:

- 1- Goal and systems definition, in which the system's flows and stocks should be defined and system boundaries (in terms of space and time) established according to the aim of the study,
- 2- System flows and stocks quantification, in which the system should be quantified through either accounting or modelling,
- 3- Interpretation of the results, in which the overview of the system flows and stocks is transformed into policy relevant information.

SFA is based on the principle of materials balance, which enables different types of analysis. Substance flow accounts can be used to identify major flows and accumulations and to spot trends. Static models can be used to identify the causes of pollution problems and to assess the effectiveness of contra-measures (Baccini and Bader, 1996 and van der Voet, 1996a). Dynamic models allow the exploration of future flows and stocks (resources, emissions and wastes) (Bergback and Lohm, 1997) and provide a relevant input for strategic environmental policy planning.

In SFA, the system is treated as a physical entity: a coherent set of elements that determine the flows of a certain substance or group of substances. Generally, the SFA system represents a geographically demarcated area: a country, region, group of countries, or even the whole world. In most cases, the SFA system is divided in two subsystems, the economic and the environmental. The economic subsystem is also called the 'societal subsystem', 'technosphere' or 'anthroposphere' – indicating that the system is not concerned with financial aspects. The environmental subsystem is also referred to as the biosphere.

The outcomes of SFA models can be transferred into policy relevant information. SFA is a useful tool for identifying potentially problematic substances at an early stage, for example in identifying the causes of pollution problems, assessing the necessity of action, the effectiveness of contra-measures and forecasting future developments. In this way it can provide an early warning of future problems.

SFA case studies have been carried out at a wide range of spatial levels: the international (Voet et al., 1994, Lanzano et al., 2006, Spatari, et al., 2003), national (Antikainen, et al., 2004, Tasaki, et al., 2004), and local and company levels (Burström, 1999, Lindqvist and Malmberg, 2004, Timmermans and Van Holderbeke, 2004, Van Holderbeke and Timmermans, 2002, Nilsson, 1995). SFA has proven to be particularly useful in spotting unintended flows: the occurrence of the substance as a trace contaminant in materials derived from fossil fuels, phosphate rock etc. (Guinée et al., 1999).

SFA can also be used as a basis for subsequent analysis. Environmental fate modelling is considered as a specific form of SFA. These models, which focus on environmental flows, are based on the physical and chemical properties of substances and environmental characteristics (Van der Voet et al., 2000). These models can be used as a starting point for risk analysis.

## 2.4 Modelling flows and stocks in SFA

The second element of the SFA framework, the one to which this thesis will mainly contribute, involves the description of the relations between flows and stocks in the economic subsystem. As discussed above, there are several aspects to such modelling. This section focuses on two main types: static and dynamic.

Static SFA models describe system flows and stocks, and present them as dependent on one another, through a set of linear equations that can be solved for a specific year by assuming a stationary state, i.e. one in which the flows do not change over time. The system is described in terms of nodes, sources and sinks. Flows can be fixed, determined by model relations, or provided by balancing equations. Static models, require a limited number of fixed flows and the outcome relies mainly on the distribution pattern implying that data are required on the production and environmental processes and the way substance flows are redirected by them (Van der Voet, 1996a). Although static models are more limited than dynamic models, they do have several advantages. They require far less data and the outcome is more robust, due to the exclusion of many uncertainties. Several static SFA models have been developed and applied to various substance groups, including heavy metals (Van der Voet, et al., 1994, Van der Voet, 2000), nutrients (nitrogen and phosphorous) (Schröder, 1995, Van der Voet et al., 1996b, Van der Voet et al., 1996c, Nilsson, 1995, Antikainen, et al., 2004), and chlorine (Kleijn et al., 1993, Kleijn et al., 1997, Tukker et al., 1997).

Dynamic SFA models take into account changes in system flows and stocks over time. The dynamic models used in this thesis are time dependent models. It has recently been recognized that one of the main difference between static and dynamic SFA models is that the latter include stocks in society. By including the dynamic behaviour of the system, it is possible to explore future flows of emissions and wastes, based on past and future inflows and stock characteristics (Kleijn et al., 2000). Taking stocks into consideration is now recognized as important, and a number of specific substance stock databases or models have been developed (Baccini, et al., 1996, Boelens & Olsthoorn, 1998; Kleijn et al., 1998, Zeltner, et al., 1999, Kleijn, et al., 2000, Binder, 2001, Voet, et al., 2002, Ayres, et al., 2003, Elshkaki, et al., 2004, Müller, et al., 2004, Elshkaki et al., 2005, Spatari, et al., 2005, Elshkaki and Van der Voet, 2006, Binder et al., 2006). The dynamics of stocks, which determine their change over time, and future flows of waste and emissions, depend on many variables. Among these are socio-economic aspects such as technological development and developments in population size, welfare, and markets. In addition to this the characteristics of substances and materials, such as degradability and volatility, also play a role: these determine emissions during use, corrosion, life span, recycling potential etc..

The future emission and waste flows from society to the environment can be described through two different forms:

- 1- The leaching model, in which the concentration of the substance is the driving force (e.g. the leaching of copper from water pipes through corrosion). In this case the outflow is described as a fraction of the stock.
- 2- The delay model, in which the age is the driving force (e.g. the generation of waste containing copper from discarded products). In this case the outflow is described as a delayed inflow.

Two approaches can be used to model the stock that is in use, the inflow of substances into the stock and the outflow of substances from the stock.

The first approach starts from historical data on the inflow into the stock and the product lifetime to estimate the past and future outflow from the stock and the stock-in-use (Baccini, et al., 1996, Zeltner, et al., 1999, Kleijn, et al., 2000, Van der Voet, et al., 2002, Ayres, et al., 2003, Elshkaki, et al., 2004, Elshkaki et al., 2005, Spatari, et al., 2005, Elshkaki and Van der Voet, 2006, Binder et al., 2006). For the future, the inflow into the stock-in-use is either assumed (Kleijn, et al., 2000) or estimated based on socio-economic variables using different techniques, such as intensity of use and regression analysis (Elshkaki et al., 2004). The second approach starts from historical data on the stock-in-use and the product lifetime to estimate the past and future outflow and the future inflow (Binder, 2001, Elshkaki, et al., 2004, Müller, et al., 2004). The future stock is related to the service provided by the product and estimated based on socio-economic variables (Elshkaki et al., 2004, Müller, et al., 2004).

## 2.5 Software tools

A crucial aim of modelling the dynamic behaviour of systems is to improve understanding of the system elements and actors and how these affect the system's behaviour, thus enabling better forecasts.

In the mathematical and statistical world, several techniques are available for analysing dynamic systems. A few of these have been used in the field of Substance Flow Analysis (Kleijn et al. 2000). Software tools are an important aid in the successful implementation of such mathematical and statistical modelling techniques. These software tools can play an important role in SFA models. They facilitate the organising and analysing of data, deal with uncertainty, and are useful in modelling, and calculating (standardised) performance indicators. Moreover, they provide the possibility for scenario analysis, graphical presentation of the systems and the possibility of linking to other types of models.

A number of models have been developed and dedicated to substances and products analysis tools - SFA, MFA and LCA (Boelens & Olsthoorn, 1998). These software models can run on a PC under the ms-dos or Microsoft Windows platforms. These vary in their purposes and structures and include (to mention just a few): SFINX (Van der Voet, 1996a), SIMBOX (Baccini and Bader, 1996), ORWARE (Dalemo et al., 1997), FLUX (Olsthoorn and Boelens, 1998 and Boelens and Olsthoorn, 1998), DYNFLOW (Elshkaki, 2000), GaBi (IKP and PE Europe GMBH, 2006) and UMBERTO (IFU, 2006).

To date the existing SFA software tools have focused on the static, linear or non-linear, types of modelling. Dynamic modelling has mostly been neglected or inadequately included. Yet there are many well-known systems dynamic modelling software packages, including SIMULINK, STELLA, POWERSIM, and VENSIM. These can enhance the modelling and the simulation of complex dynamic systems.

Some of these software packages have been used to model ecological and economic systems such as STELLA, and VENSIM (Costanza and Gottlieb, 1998 and Ford, 1999) and others such as MATLAB and its extension SIMULINK, have been used to model environmental and technical systems (Eriksson et al., 2002 and Kumblad et al., 2003).

The software model used in this thesis uses MATLAB and SIMULINK as a starting point. They were chosen for several reasons. SIMULINK is an advanced extension of MATLAB software that assists in modelling, simulating, and analysing complex dynamic systems. It supports linear and non-linear systems, modelled in continuous time, sampled time or a hybrid of the two. SIMULINK provides features such as block libraries, hierarchical modelling, signal labelling, and subsystem masking, which makes it a powerful dynamic systems simulation tool. Its block library consists of over one hundred blocks. These are grouped into libraries according to how they function in the system. These blocks are the basic elements from which SIMULINK models are built. The user can model virtually any dynamic system by creating and interconnecting blocks in appropriate ways. SIMULINK provides a graphical user interface for building models as block diagrams, using click and drag mouse operations. With this interface, users can draw the model as they would with pencil and paper. The visual block diagram interface offers a simple method for constructing, modifying and maintaining complex system models. The user can also create custom blocks in two programming languages, C++ and FORTRAN, and add them to the SIMULINK block library. SIMULINK provides a convenient feature for customizing subsystem blocks, called masking. It gives a high degree of flexibility for customizing the SIMULINK modelling environment, as well as the behaviour and user interface of any block.

Although SIMULINK requires programmers to provide additional model structures that can be automatically created in other software, this gives them more control over specific aspects in the modelling process. For example, if a parameter needs to be estimated by using a value that should be lagged in time, circular dependencies appears in other dynamic software packages (Rizzo et al., in press).

A new software tool, called DYNFLOW, which is based on MATLAB and its extension SIMULINK has recently been developed by Elshkaki (2000). DYNFLOW is dynamic system software for substance flow analysis. It combines a dynamic modelling core with a user friendly interface and possibilities for graphical presentation. DYNFLOW uses the features of SIMULINK to not only model dynamic SFA models but also to structure and model static SFA cases (Elshkaki, 2000).

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## **Chapter 3    Dynamic Substance Flow-Stock Model**

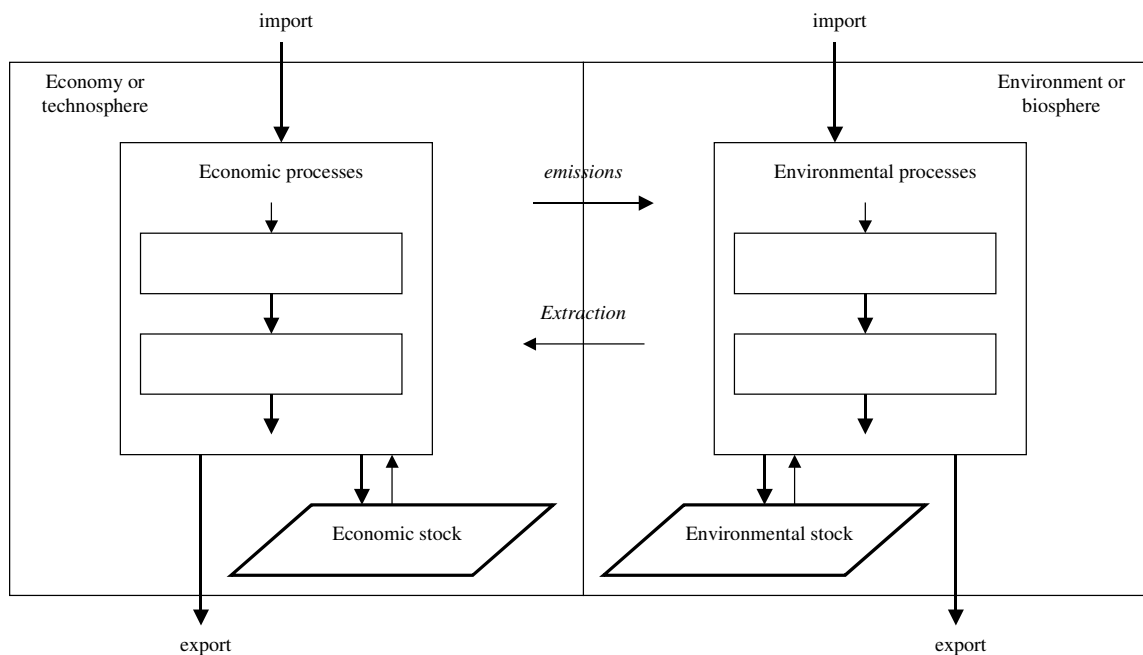
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### 3.1 Introduction

Within the community of systems analysis, there are many interpretations of what a system is. In general, the term ‘system’ can be defined as a group of interacting, interrelated or interdependent elements forming a complex entity. Each element has specific properties that enable the system to function. A system can be a physical or social entity, or an abstract idea, and can be either open or closed.

In Substance Flow Analysis, the system is a physical entity, which is divided in two subsystems, the economic and the environmental. Sometimes, it is not clear where exactly to draw the border between the two. A landfill is situated in the environment but is still under human control. However, the choice of treating a landfill as part of the environment or of the economy will not make any difference in modelling terms or to the outcome of the SFA model. This is in contrast to, for example, LCA where the boundary between the technical subsystem and the environment has to be drawn as one of the system boundaries (Guinée et al., 1993), as it determines what to call “emissions”. It is generally accepted that the emissions from landfill sites should be included in the inventory and therefore that the landfill sites should be included in the economic subsystem (Heijungs et al, 1992 & Finnveden et al, 1995). Likewise, agricultural soil may be treated as an environmental component or as part of the economic subsystem, due to the fact that it is also used as a mean of production.

The economic and the environmental subsystems are shown in figure 1. The economic subsystem includes several processes (extraction, production, consumption and waste management processes) and several flows and stocks. Economic stocks are contained in the production and consumption phases, landfill sites, and agricultural soil. The environmental subsystem includes several processes (leaching, evaporation and deposition), and also contains several flows and stocks. Environmental stocks are those in the non-agricultural soil and natural resource stock. The environmental components in the model are air, water and non-agricultural soil.



**Fig. 1:** The economic and the environmental subsystems and their components



SFA studies typically cover a period of one year. Flows of goods appear within this year and goods are transferred from one process to another. In the use phase, goods with a life span of longer than 1 year tend to accumulate: they do not flow out in the same year but remain for longer in the use-process. Such applications, with a life span of more than 1 year, are referred to as stocks. Although SFA typically covers a period of one year, a shorter time period can also be used (e.g., one month, one day, etc.). Goods with a life span longer than the time period taken in the model will be accumulating. This study uses a time period of one year.

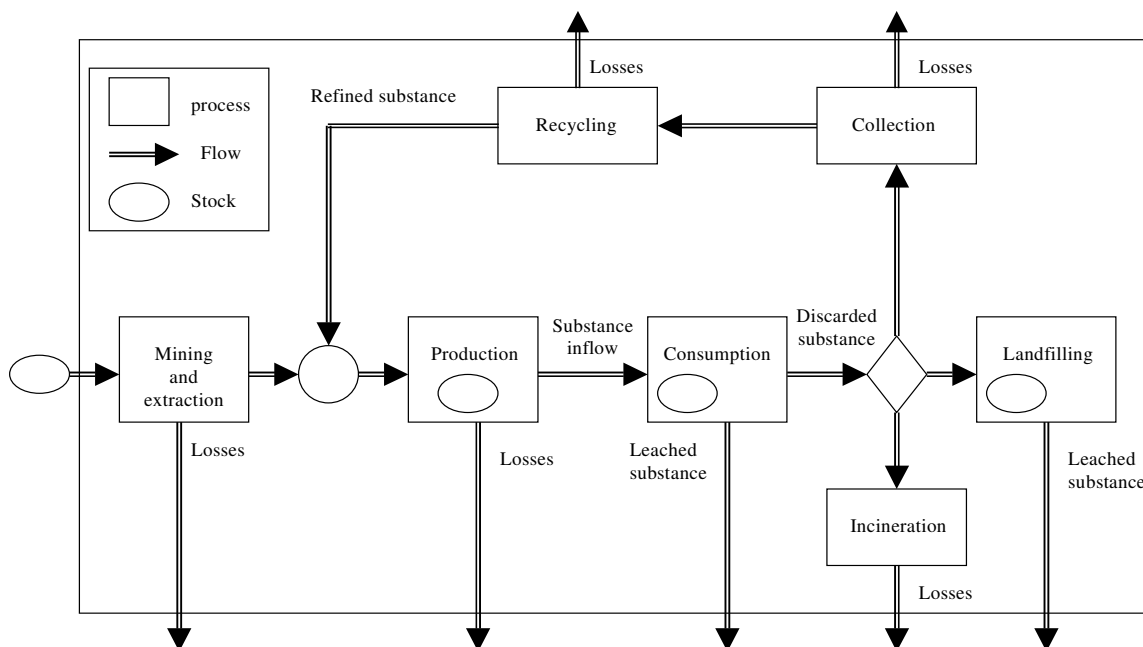
SFA always focuses on investigating a specific substance. All flows and stocks therefore are regarded in terms of the substance as a chemical element and are specified in these terms. A substance may occur in a number of materials and in an even larger number of products. A substance stock therefore includes materials stocks, which in turn include product stocks. A careful distinction needs to be maintained between the stock of products, handled by producers and consumers, the stock of materials that those products are composed of, and the stock of a substance, contained within these products and materials and eventually resulting in emissions. The stock dynamics can be a result of developments at all three levels.

In the following sections, the economic and the environmental subsystems, their main components, their main variables and parameters and the most important aspects affecting their dynamic behaviour will be discussed.

## 3.2 Economic subsystem

### 3.2.1 General

The economic subsystem has three main component categories: processes, flows, and stocks. The flows and stocks represent certain economic goods. Flows refer to goods travelling from one process to another. Stocks are goods stored within the economic subsystem. Goods are transformed from one state to another through the processes. When this transformation takes place within the time period taken in the model (here one year), the goods will appear as flows in the SFA system. If this transformation takes a longer time, the goods will appear as stocks. Processes, flows and stocks in the economic subsystem are shown in figure 2.



**Fig. 2:** The main processes, flows, and stocks in the economic subsystem.

### *Categories of processes*

**Mining and extraction**, the processes through which raw materials are extracted from the biosphere or geosphere and transformed into materials that can be used in production and manufacturing. **Production and manufacturing**, the processes through which raw materials are transformed into finished goods. **Transportation**, the processes of transporting goods from one place to another, which does not involve any transformation. **Consumption and use**, the processes through which products are transformed into discarded products. These may involve a considerable time period. **Hibernation**, the processes involving storage of products no longer in use, but not yet discarded. **Waste treatment**, the processes involving the treatment of waste materials, thereby transforming discarded products into re-used products, recovered energy, recycled materials, landfilled waste, or emissions.

### *Categories of flows*

**Mined raw materials**, the extraction or mining from the environment of a flow of raw materials containing the substance under study, which then enters into the economic subsystem. **Products**, the flow of different kinds of finished goods containing the substance into the consumption phase, either through production processes within the studied system or entering it through trade. **Discarded products**, the flow of discarded goods from the consumption and/or hibernating phases to the waste-processing phase. **Reused products/recycled materials**, the flow of goods recaptured from the waste stream and returned to the production or consumption phases. **Final waste**, the flow of materials with no economic value to be disposed of. At present disposal is either through landfill or incineration. Ashes and slag from the incineration process may be recycled or end up in landfill. Materials may also be emitted to the environment. **Emissions**, the flow of materials or substances from the economic subsystem to the environmental subsystem. Emissions represent losses from processes in the economic subsystem through corrosion, leakage or volatilization and can occur in all phases of the life cycle. The emissions themselves are not intended. By making changes to certain processes, they can be intentionally reduced or prevented. **Imported goods**, the flow of substances, materials, semi-manufactured and finished goods containing the substance entering the system under study from outside the system. These flows occur through trade with other countries or regions. **Exported goods**, the flow of substances, materials, semi-manufactured and finished goods containing the substance under study out of the system, again through trade.

### *Categories of stocks*

**Resource**, the stock of the substance in the lithosphere or biosphere. **Product and material stock in industries**, the stock of goods and materials containing the substance under study kept in industries or in storage prior to use. **Product stock in use**, the stock of goods in use, containing the substance under study providing the service they were made for. **Hibernating products**, the stock of goods containing the substance under study that no longer provide the service they were made for but not yet discarded. **Substance stock in use**, the stock of the substance under study in the use phase. **Landfilled waste**, that is, the stock of final waste deposited at landfill sites.

The modelling of these processes flows and stocks in the economic subsystem will be described in the next sections. The starting point for the modelling is the consumption of applications containing the substance, mainly the demand for the substance being studied. Other aspects of the economic subsystem are mainly derived from this.

## **3.2.2 Consumption of substance- containing applications**

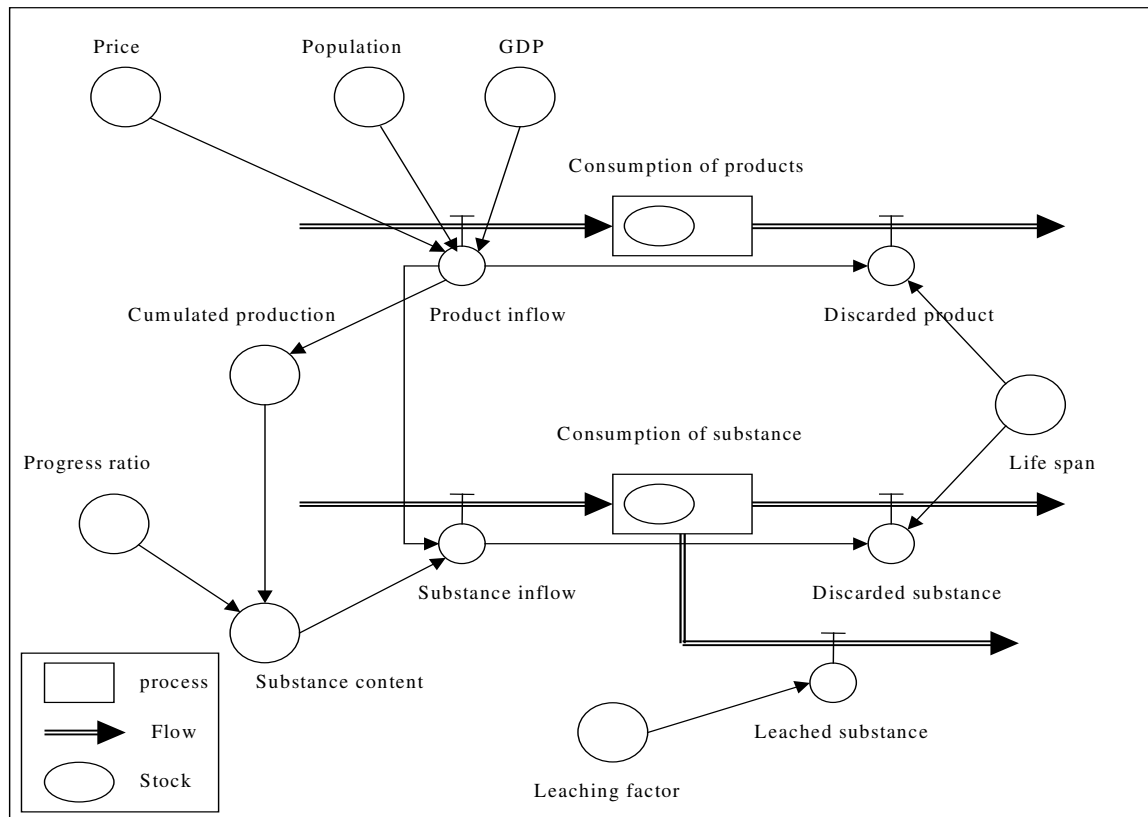
In general, the stock of a substance or material consists of all the products containing the substance or material that have a life span that exceeds the time period used in the model (1 year). This can involve a large number of products with widely differing characteristics. This implies that a substance stock model should contain two levels: the substance level and the product level, as shown in figure 3. Products have a given demand and life span, which may or may not be influenced by the substances it contains. A substance in a product may be substituted without changing the demand for the product. The substance in a waste

product may be extracted and recycled, and subsequently used in different products. In this scenario the substance leaves the specific product stock but not society, and the life span of the substance may differ considerably from that of the applications in which it used.

### 3.2.2.1 Modelling the inflow of substances into the stock-in-use

The inflow of a substance into a stock-in-use is determined by the demand for products containing the substance and the substance content of products. The demand is influenced by socio-economic and economic factors such as Gross Domestic Product (GDP), per capita GDP, population size and growth, inter and intra-sectoral shares in GDP, price, consumer tastes and preferences, the possibilities of substitution and technical developments.

The model employs two approaches to model the inflow of a substance into the stock-in-use. In some cases the inflow of substances is modelled on the inflow of products multiplied by their substance content. In these cases the inflow of products and the inflow of the substance are modelled using two separate equations, determined by different factors as shown in figure 3.



**Fig. 3:** The inflow of a substance into the substance stock-in-use, based on the product/substance approach

In the model, Eq. 1 is used to determine the inflow of products into the stock-in-use and is then multiplied by the substance content as given by Eq. 2. A regression model is used to establish the relative importance of the independent variables on the shape of the inflow curve over time. The substance content can be assumed to be either constant or to change over time. If the later is assumed, the substance content can then be modelled either as a function of the cumulated production (learning curve) or as a function of time. The model adopts the learning curve concept, as given by Eq. 3 and so models the substance content as a function of the cumulated production.

$$F_{PC,i}^{in}(t) = \beta_0 + \sum_{i=1}^n \beta_i X_i(t) + \varepsilon(t) \quad (1)$$

where  $F_{PC,i}^{in}(t)$  is the inflow of product into the  $i$ th product stock at time  $t$ ,  $n$  is the number of explanatory variables,  $X_i(t)$  is the socio-economic variable at time  $t$ ,  $\beta_i$  is the model parameter and  $\varepsilon(t)$  is the model error at time  $t$ .

$$F_{C,i}^{in}(t) = SC(t) \cdot F_{PC,i}^{in}(t) \quad (2)$$

where  $F_{C,i}^{in}(t)$  is the inflow of substance into the  $i$ th product stock at time  $t$  and  $SC(t)$  is the substance content at time  $t$ .

$$SC(t) = SC_0 \cdot X(t)^{-r} \quad (3)$$

where  $SC_0$  is the initial content of the substance,  $X$  is the cumulated production and  $r$  is the experience index.

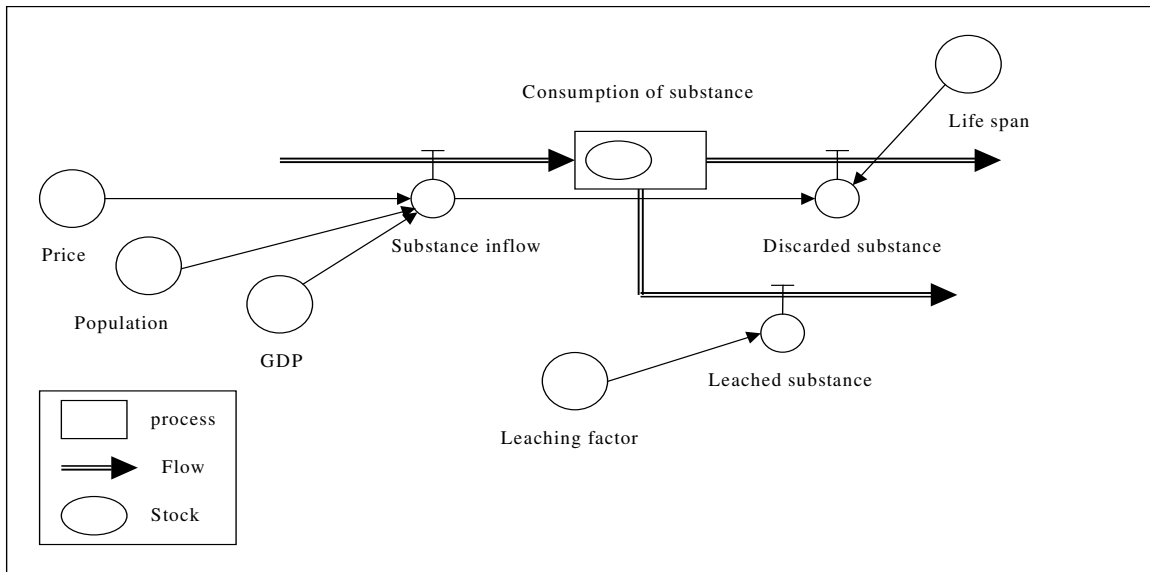
$F$ , the progress ratio, can be defined as ( $F=2^{-r}$ )

The total inflow of a certain substance into a stock-in-use is the sum of all the inflows of the substance into products in which it is used.

$$F_C^{in}(t) = \sum_{i=1}^n F_{C,i}^{in}(t) \quad (4)$$

where  $F_C^{in}(t)$  is the total inflow of the substance into the consumption phase at time  $t$

In other cases, the inflow of the substance into the stock-in-use is modelled directly (as shown in figure 4) using different types of models (linear model, log-log model and the intensity of use technique). This approach is used when the data on the substance level directly available.



**Fig. 4:** The inflow of substances into the substance stock-in-use, based on the substance approach

### 3.2.2.2 Modelling the future inflow of substances into the stock-in-use

The derived inflow model can also be used to estimate the future inflow. This requires projected values of the influential variables. Some of the explanatory variables used in modelling the inflow, such as GDP, and population are exogenously determined. Others, such as the price, can be either exogenously or endogenously determined. Projections for GDP and population are available in different scenario studies (RIVM 2000, IPCC). The assumption then is that there will be no future discontinuity in the dependency of demand on the influential variables.

#### *Approaches used to model the inflow of substances into the stock-in-use*

##### **- Linear model**

The model uses a general linear function to describe the substance inflow (the product inflow multiplied by the substance content), which is separately fitted for each product based on past trend data:

$$F_{C,i}^{in}(t) = \beta_0 + \sum_{i=1}^n \beta_i X_i(t) + \varepsilon(t) \quad (5)$$

where  $F_{C,i}^{in}(t)$  is the inflow into the  $i$ th product stock at time  $t$ ,  $n$  is the number of explanatory variables,  $X_i(t)$  is the socio-economic variable at time  $t$ ,  $\beta_i$  is the model parameter and  $\varepsilon(t)$  is the model error at time  $t$ .

The independent variables used in the model are Gross Domestic Product (GDP), Population (Pop), price (P) and a Time variable (T) that is used as a proxy for the combined influence of other variables on the inflow trend.

Sometimes the demand in a certain year does not correspond to the changes in the socio-economic variables in the same year, but to changes in these variables some years earlier. Apparently, there is sometimes a time lag between the driving forces and the response. Mathematically this time lag can be accounted for by Eq. 6:

$$F_{C,i}^{in}(t) = \beta_0 + \sum_{i=1}^n \beta_i X_i(t-j) + \varepsilon(t) \quad (6)$$

where  $X_i(t-j)$  is the socio-economic variable at time  $(t-j)$ ,  $j$  is the time lag.

##### **- Log-log model**

Another possible model to determine the inflow of a certain substance into the use phase is the log-log model (Eq. 7). The estimated coefficients of this model can be interpreted directly as elasticities.

$$\ln[F_{C,i}^{in}(t)] = \beta_0 + \sum_{i=1}^n \ln[\beta_i X_i(t)] + \varepsilon(t) \quad (7)$$

##### **- Intensity-of-use technique**

Another possible approach for modelling the inflow in the use phase is to use the intensity-of-use technique. The approach separates the impacts of the intensity of use and GDP on consumption (demand) (Tiltone). Mathematically, the relation between consumption, the intensity of use and GDP can be expressed by Eq. 8.

$$D(t) = IU(t) \cdot GDP(t) \quad (8)$$

where  $D(t)$  is the consumption (demand) at time  $t$ ,  $IU(t)$  is the intensity-of-use, and  $GDP(t)$  is the national income at time  $t$ .

The intensity of use follows a generally inverted U-shape trend (Tiltone, 1990). Although several functions can be used to capture this trend, the quadratic equation is the simplest (Roberts, 1996). The intensity of use is determined by the product composition of income, which depends on per capita income, and the material composition of products, which depends on technological change and long run price trends (Tiltone, 1990). It is possible to assume the IU as a function of per capita income (GDP/C) (Eq. 9) (Malenbaum) or as a function of time (t) (Eq. 10) (Roberts, 1996), which is used as a proxy of technological change and long run price trend. It can also be assumed as a function of both per capita income (GDP/C) and time (linear time (Eq. 11) or exponential (Eq. 12)) (Guzman, 2004).

$$IU(t) = a + b \cdot (GDP / C) + c \cdot (GDP / C)^2 \quad (9)$$

$$IU(t) = a + b \cdot t + c \cdot t^2 \quad (10)$$

$$IU(t) = a + b \cdot (GDP / C) + c \cdot (GDP / C)^2 + t \quad (11)$$

$$IU(t) = \left[ a + b \cdot (GDP / C) + c \cdot (GDP / C)^2 \right] \cdot e^{d \cdot t} \quad (12)$$

The parameters of these functions can be estimated by regression analysis

### 3.2.2.3 Modelling the leaching outflow of substances from the stock-in-use

The outflow of substances out of the stock takes place through two processes: leaching and delay (Van der Voet et al. 2002). Leaching occurs during use, due to corrosion or slow volatilization of substances from various stocks of applications. These emissions may end up in the soil, surface water, ground water or sewage system. The yearly emissions of a substance in a certain application can be modelled as a fraction of the total size of the stock by using linear or exponential emission coefficients. The model uses a linear emission coefficient, as given by Eq. 13.

$$F^{out}_{C,E,i}(t) = \alpha_i \cdot S_{C,i}(t) \quad (13)$$

where  $F^{out}_{C,E,i}(t)$  is the outflow due to emissions at time t,  $\alpha$  is the emission factor and  $S_{C,i}(t)$  is the stock of the substance in product i at time t.

### 3.2.2.4 Modelling the delayed outflow of substances from stock-in-use

Delay is related to the discarding of products after use. The discarded outflow of a product depends mainly on the product inflow and its life span. Empirical data on the life span is often not available and as an alternative one can either assume an average life span or a certain life span distribution.

The discarded outflow can be modelled as a delayed inflow, corrected for emissions that occur during use, as given by Eq. 14:

$$F^{out}_{C,D,i}(t) = F^{in}_{C,i}(t - L_U) - \sum_{i=1}^{L_U} \alpha_i \cdot F^{in}_{C,i}(t - L_U) \cdot (1 - \alpha_i)^{i-1} \quad (14)$$

where  $F^{out}_{C,D,i}(t)$  is the outflow due to the delay mechanism at time t,  $\alpha$  is the emission factor and  $L$  is the average life span of the product.

Or in the case of using a Weibull distribution, the discarded outflow at time t is a weighted sum of all past values of the inflow up to the present time, as given by Eq. 15.

$$F^{out}_{C,D,i}(t) = \sum_{j=0}^{\infty} W_j \cdot F^{in}_{C,i}(t-j) = \sum_{j=-\infty}^t W_{t-j} \cdot F^{in}_{C,i}(j) \quad (15)$$

where the lag weights  $w$  are the probabilities of exiting the delay in any time period  $j$  and must sum to unity.

$$\sum_{j=0}^{\infty} W_j = 1$$

The total outflow at time  $t$ ,  $F^{out}$  is given by Eq. 16.

$$F^{out}_{C,i}(t) = F^{out}_{C,D,i}(t) + F^{out}_{C,E,i}(t) \quad (16)$$

The use of the delay model requires intensive historical information. In some cases it is possible to use the leaching model, which requires less information, as a proxy for the delay model (Van der Voet et al. 2002) using  $\alpha_i = 1/L_{ui}$ . To use the leaching model as an approximation of the delay model, it must be possible to describe the inflow curve by an exponential function, the life span ( $L$ ) is short and the parameter describing the direction and the steepness of the graph is small.

For some applications, use is sometimes equal to the emissions to the environment. This is the case with the lead applied in ammunition: once the bullets are used, lead is brought directly into the environment. In cases like this, an explicit borderline between the economy and the environment has to be made: Is the bullet, once shot, the emission, or is the emission only the corrosion once it is laying on the soil?

### 3.2.2.5 Modelling substances stock-in-use

The change of the magnitude of the stock over time is the difference between the inflow and the outflow, as given by the differential equation (Eq. 17).

$$\frac{dS_{C,i}}{dt} = F^{in}_{C,i}(t) - F^{out}_{C,i}(t) \quad (17)$$

where  $F^{in}_{C,i}(t)$  is the inflow into the  $i$ th product stock at time  $t$ ,  $F^{out}_{C,i}(t)$  is the outflow from the  $i$ th product stock at time  $t$  and  $S_{C,i}$  is the  $i$ th product stock.

### 3.2.2.6 Modelling hibernating stock

The term "hibernating stock" refers to the stock of goods no longer providing the service they were made for, but not yet discarded. Some goods are stored for some time before being discarded. The main difference between the stock-in-use and the hibernating stock lies in the product life span. In the use phase, the life span is determined by the technical specification of the product. In the hibernating phase, however, the life span is determined by the consumer's decision. If a product is stored before being discarded, this hibernating time should be taken into account, either by adding the hibernating time ( $L_H$ ) to the use time ( $L_U$ ), if the entire discarded outflow enters the hibernating stock, or by modelling the hibernating phase separately. If the hibernating phase is to be modelled separately, the change of the magnitude of the hibernating stock is the difference between its inflow and outflow as given by Eq. 18.

$$\frac{dS_{H,i}}{dt} = F^{in}_{H,i}(t) - F^{out}_{H,i}(t) \quad (18)$$

where  $F^{in}_{H,i}(t)$  is the inflow into the hibernating stock at time  $t$  and  $F^{out}_{H,i}(t)$  is the outflow from the hibernating stock at time  $t$ .

The inflow into the hibernating stock ( $F_{H,i}^{in}$ ) is the discarded outflow of the stock-in-use ( $F_{C,D,i}^{out}$ ), or part of it, as given by Eq. 19.

$$F_{H,i}^{in}(t) = \alpha_{H,i} \cdot F_{C,D,i}^{out}(t) \quad (19)$$

where  $\alpha_{H,i}$  is the fraction of the discarded outflow of the stock-in-use which enters the hibernating stock.

The outflow from the hibernating stock is the outflow due to the emissions during hibernation ( $F_{H,E}^{out}$ ) and the discarded outflow ( $F_{H,D}^{out}$ ). The same mathematical equations used for modelling the outflow from the stock-in-use (Eqs. 13 and 14) can be used.  $L_U$  in Eq. 14 should be replaced by the hibernating time ( $L_H$ ). Alternatively, Eq. 14 can be employed directly, with the life span being the use life span plus the hibernating life span.

### 3.2.3 Mining and co-production of substances

#### 3.2.3.1 Mining and extraction of substances

The total amount of a substance taken from ore is determined by the amount required from primary production and emissions of the substance during the production processes.

$$F_p^{in}(t) = F_p^{out}(t) + [\alpha \cdot F_p^{out}(t)] = (1 + \alpha) \cdot F_p^{out}(t) \quad (20)$$

The amount of a substance required from primary production is determined by the total demand for the substance (the flow of the substance into the production processes) and the available amount of secondary materials.

$$F_p^{out}(t) = F_{pp}^{in}(t) - [\alpha \cdot F_{R,R}^{out}(t)] \quad (21)$$

where  $F_p^{in}$  is the inflow of substances into primary production processes (the extracted flow) and  $F_p^{out}$  is the outflow from these processes (refined primary substances)

The outflow of secondary materials from recycling processes is either partly or completely used in producing new products. This is mainly determined by the price of secondary material compared to the price of primary material on the world market.

#### 3.2.3.2 Co-production of substances

The amount of co-produced substances is estimated from the required primary production of the main substance and the co-produced material content of the ores.

$$F_x^{in}(t) = \alpha_x \cdot F_p^{in}(t) \quad (22)$$

where  $F_{x(t)}^{in}$  is the inflow of the co-produced substance into the economy at time t,  $F_{p(t)}^{in}$  is the inflow of the substance into primary production processes at time t, and  $\alpha_x$  is the ratio between the substance and co-produced substance.

### 3.2.4 Production of substance-containing applications

#### 3.2.4.1 Modelling the inflow of substances into the production processes

The total inflow of a substance into the production processes is the amount needed to produce the different required products, as given by Eq. 23.



$$F_{PP}^{in}(t) = \sum_{i=1}^n F_{PP,i}^{in}(t) \quad (23)$$

$F_{PP}^{in}(t)$  is the total inflow of a substance into the production processes of all the applications at time  $t$ ,  $F_{PP,i}^{in}(t)$  is the inflow of the substance into the production process of product  $i$  at time  $t$  and  $n$  is the number of products.

For each application, the inflow of the substance into the production process is equal to the outflow of the substance in the produced product plus the other outflows from the production process (emissions to air and water, and waste flow), as given by equation 24.

$$F_{PP,i}^{in}(t) = F_{PP,i,P}^{out}(t) + F_{PP,i,A}^{out}(t) + F_{PP,i,W}^{out}(t) + F_{PP,i,L}^{out}(t) \quad (24)$$

$F_{PP,i}^{in}(t)$  is the inflow of the substance into the production process of product  $i$  at time  $t$ ,  $F_{PP,i,P}^{out}(t)$  is the outflow of the substance in the produced product  $i$  at time  $t$ ,  $F_{PP,i,A}^{out}(t)$  is the outflow of the substance to the air during the production process of product  $i$  at time  $t$ ,  $F_{PP,i,W}^{out}(t)$  is the outflow of the substance to the water during the production process of product  $i$  at time  $t$ , and  $F_{PP,i,L}^{out}(t)$  is the outflow of the substance to the landfill sites from the production process of product  $i$  at time  $t$ .

The inflow of the substance into the production process of product  $i$  ( $F_{PP,i}^{in}$ ) is estimated directly for each product as a balancing item of the production process as given by Eq. 29. The total inflow of the substance  $F_{PP}^{in}$  is estimated in Eq. 23. This implies that it is not supply, but demand (i.e. domestic and foreign demand for products containing the substance) that is the driving force.

### 3.2.4.2 Modelling the outflow of substances from production processes

The total outflow of the substance from the production processes is the combination of the substance in the produced products, the emissions from the production processes, and the waste flow to landfill. If the modelled system is large (global), imports and exports can be neglected. Consequently the outflow of the substance into the produced products is equal to the inflow of the substance into the stock-in-use (Eq. 25).

$$F_{PP,i,P}^{out}(t) = F_{C,i}^{in}(t) \quad (25)$$

The other outflows can be estimated as a fraction of the outflow of the substance in products as given by Eqs. 26, 27 and 28.

$$F_{PP,i,A}^{out}(t) = \alpha_{PA,i}(t) \cdot F_{PP,i,P}^{out}(t) \quad (26)$$

$$F_{PP,i,W}^{out}(t) = \alpha_{PW,i}(t) \cdot F_{PP,i,P}^{out}(t) \quad (27)$$

$$F_{PP,i,L}^{out}(t) = \alpha_{PL,i}(t) \cdot F_{PP,i,P}^{out}(t) \quad (28)$$

where  $\alpha_{PA,i}(t)$  is the air emission factor at time  $t$ ,  $\alpha_{PW,i}(t)$  is the water emission factor at time  $t$  and  $\alpha_{PL,i}(t)$  is the landfill factor at time  $t$ .

### 3.2.4.3 Modelling the stock in production processes

In the production phase of the applications containing the substance in question, the change of the magnitude of the substance's stock over time is assumed to be 0, as given by Eq. 29. Therefore, the inflow of substances into the production of different applications is equal to the total outflow from the production processes (emissions and products).

$$\frac{dS_{PP,i}(t)}{dt} = 0 = F_{PP,i}^{in}(t) - F_{PP,i}^{out}(t) \quad (29)$$

where  $F_{PP,i}^{in}(t)$  is the total inflow of a substance into the production processes of each application at time  $t$ , and  $F_{PP,i}^{out}(t)$  is the total outflow of a substance from the production processes of all applications at time  $t$ .

### 3.2.5 Waste management of substance containing applications

Part of the discarded outflow ( $F_D^{out}$ ) from the stock-in-use and/or the hibernating stock will be collected for recycling purposes and part will end up in final waste treatment, either on landfill sites or in incineration plants. Collected, incinerated and landfilled streams are modelled as fractions of the discarded outflow as given by Eqs. 30 and 31. Figure 5 shows the main factors determining the distribution of the substance in the waste management phase.

$$F_{SC,i}^{in}(t) = a_1(t) \cdot F_{C,D,i}^{out}(t) \quad (30)$$

$$F_{inc,land,i}^{in}(t) = F_{inc,DC,i}^{in}(t) + F_{land,DC,i}^{in}(t) = F_{C,D,i}^{out}(t) - F_{SC,i}^{in}(t) \quad (31)$$

Where  $F_{SC,i}^{in}(t)$  is the amount of scrap waste material collected for recycling purposes, at time  $t$  and  $a_1(t)$  is the collection rate.  $F_{inc,land,i}^{in}$  is the inflow of the substance into incineration plants and landfill sites from the discarded product  $i$ ,  $F_{inc,DC,i}^{in}$  is the inflow of the substance into incineration plants from the discarded product  $i$ , and  $F_{land,DC,i}^{in}$  is the inflow of the substance into the landfill sites from the discarded product  $i$ .

#### 3.2.5.1 Collection

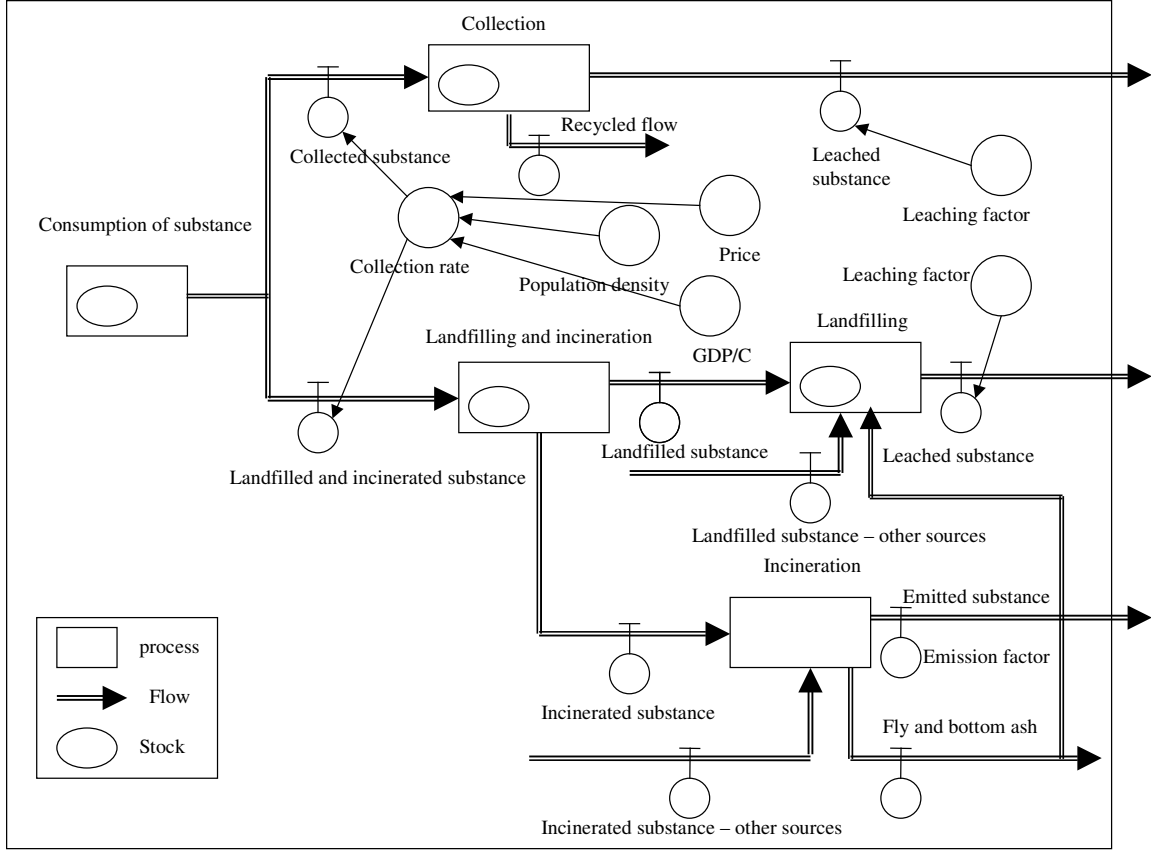
In this phase the collected part(s) from obsolete products are gathered and stored for some time before entering the recycling processes.

##### *The inflow of substances into the collection phase*

The inflow of substances into the collection phase is a fraction of the discarded outflow from the stock-in-use and/or the hibernating stock. The stream of collected materials is mainly determined by policy, economic, technical and socio-economic aspects.

Economic factors, largely derived from the ratio of primary and secondary material prices, are the main determinants of the extent to which the recycling process is profitable. The price of secondary material can be used as a proxy for the cost involved at this phase (the cost of collection and transportation). The model can test and regulate the effects of policy through applying different policy measures, such as a landfill tax. The socio-economic and demographic factors are indicated by per capita GDP and population density.

Regression analysis is used to parameterise the relation between the collection rate ( $a_1$  in Eq. 30) of each of the substance's applications and the different factors that influence this (the cost of collection and transport, population density, per capita GDP, Landfill tax, etc.). A general function similar to Eq. 1 is used to describe the collection rate. This can be fitted separately to each product according to the past collection rate trend data.



**Fig. 5:** The distribution of a substance between different waste management options

### *The outflow of substances from the collection phase*

The outflow from the collection phase is due to emissions during storage time and the flow of substances entering recycling processes, as given by Eq. 32.

$$F_{SC,i}^{out}(t) = F_{SC,i,E}^{out}(t) + F_{SC,i,R}^{out}(t) \quad (32)$$

$F_{SC,i}^{out}(t)$  is the outflow from the collection phase at time  $t$ ,  $F_{SC,i,E}^{out}(t)$  is the emitted outflow at time  $t$  and  $F_{SC,i,R}^{out}(t)$  is the outflow going to recycling processes at time  $t$ .

The outflow to the recycling processes can be estimated as delayed inflow, by using an equation similar to Eq. 14. The storage time could range from 0 to a few years. The outflow due to the emissions during storage time can be estimated as a fraction of the stock using an equation similar to Eq. 13.  $\alpha$  in Eq. 13 is the emission factor and  $L$  in Eq. 14 is the storage time of obsolete products in this phase.

### *Substance stock in the collection phase*

The change in the magnitude of stock of the substance in the collection phase over time is the difference between the inflow (the part collected from obsolete products) and the outflow (the emitted outflow during storage time and the recycled flow) as given by Eq. 33.

$$\frac{dS_{SC}(t)}{dt} = F_{SC,C}^{in}(t) - F_{SC}^{out}(t) \quad (33)$$

$S_{sc}$  is the stock of substance in the collection phase,  $F_{sc}^{in}$  is the inflow of the substance collected from obsolete products and  $F_{sc}^{out}$  is the outflow of the substance in obsolete products to recycling processes and emissions during storage.

### 3.2.5.2 Recycling

Recycling materials involves several interconnected processes. The recycling process begins with the collection of obsolete products, followed by sorting and separation activities and finishing (in the case of metals) with smelting and refining processes. Each process has its own requirements (material, energy), recoveries and losses (waste and emissions).

The recycling industry is driven by market-based factors, such as the cost of the different processes and the price of primary material compared to secondary material.

#### *Inflow to the recycling processes*

If the modelled system is large (global), the imports and exports can be disregarded. Consequently  $F_R^{in}$  can be estimated, as given by Eq. 34.

$$F_R^{in}(t) = F_{SC,R}^{out}(t) \quad (34)$$

#### *Outflow from the recycling processes*

The outflow from recycling processes is emissions during these recycling processes, the waste flow to landfill, the waste flow used for other applications (non-intentional flows of substance) and the useable secondary materials, as given by Eq. 35.

$$F_R^{out}(t) = F_{R,E}^{out}(t) + F_{R,W}^{out}(t) + F_{R,CNI}^{out}(t) + F_{R,R}^{out}(t) \quad (35)$$

$F_R^{out}(t)$  is the total outflow of the substance from recycling processes at time  $t$ ,  $F_{R,E}^{out}(t)$  is the emitted outflow at time  $t$ ,  $F_{R,W}^{out}(t)$  is the landfilled outflow at time  $t$ ,  $F_{R,CNI}^{out}(t)$  is the waste outflow used in other applications (non-intentional applications) at time  $t$  and  $F_{R,R}^{out}(t)$  is the substance secondary outflow at time  $t$ .

Each of the outflows from recycling processes can be estimated as a fraction of the outflow of secondary materials as given by Eqs. 36, 37 and 38.

$$F_{R,A}^{out}(t) = \alpha_{RE}(t) \cdot F_{R,R}^{out}(t) \quad (36)$$

$$F_{R,L}^{out}(t) = \alpha_{RL}(t) \cdot F_{R,R}^{out}(t) \quad (37)$$

$$F_{R,CNI}^{out}(t) = \alpha_{CNI}(t) \cdot F_{R,R}^{out}(t) \quad (38)$$

$F_{R,R}^{out}(t)$  is the outflow of secondary materials from recycling processes within the country at time  $t$  and  $\alpha's(t)$  are the emission, landfilled waste and used waste factors at time  $t$ .

#### *The stock of substances in recycling processes*

The phase of recycling includes the sorting, smelting and refining of obsolete products. The change of the magnitude of the stock over time is assumed to be 0, as given by Eq. 39. Therefore, the inflow of obsolete products to recycling processes (the outflow from the collection phase) is equal to the outflow from the recycling processes (emissions, waste and useable secondary materials).

$$\frac{dS_R(t)}{dt} = 0 = F_R^{in}(t) - F_R^{out}(t) \quad (39)$$

### 3.2.5.3 Incineration

#### *The inflow of substances into incineration plants*

The inflow of substances into incineration plants mainly comes from the stock-in-use of different substance applications. For each application this flow is estimated in combination with the inflow of substances to be landfilled and is calculated as the difference between the total discarded waste stream from the stock-in-use of these applications and the flow collected for recycling, as given by Eq. 31.

The inflow of substances into incineration plants from discarded products is estimated as a fraction of the total uncollected flow for each product, as given by Eq. 40. This fraction is determined by several factors, including policy and the characteristics of the waste stream. The model can employ different scenarios to estimate the inflow of substances into incineration plants.

$$F_{inc,DC,i}^{in}(t) = \alpha_{1,i}(t) \cdot F_{inc,land,i}^{in}(t) \quad (40)$$

$\alpha_{1,i}$  is the fraction of the total uncollected flow of product  $t$  that ends up in incineration plants

The total inflow of substances into incineration plants is the inflow of substances from discarded products and the inflow from other sources, as given by Eq. 41.

$$F_{inc,t}^{in}(t) = \sum_{i=1}^n F_{inc,DC,i}^{in}(t) + F_{inc,others}^{in}(t) \quad (41)$$

where  $F_{inc,others}^{in}$  is the inflow of substances into incineration plants from sources other than discarded products.

Other inflows into incineration plants such as that of incinerated sewage sludge are estimated as model relations.

#### *The outflow of substances from incineration plants*

The total outflow of substances from incineration plants is equal to the inflow of these substances into incineration plants. The outflow of substances from incineration plants is contained in incineration residues (bottom and fly ash) and emissions from incineration (Eq. 42). Each of these outflows is estimated as a fraction of the total inflow of the substance into incineration plants, as given by Eqs. 43, 44, and 45. The distribution of substances between the different outflows is determined by the technical specifications of the incineration plants.

$$F_{inc,t}^{out}(t) = F_{inc,B}^{out}(t) + F_{inc,F}^{out}(t) + F_{inc,E}^{out}(t) \quad (42)$$

$$F_{inc,B}^{out}(t) = \beta_1(t) \cdot F_{inc,t}^{in}(t) \quad (43)$$

$$F_{inc,F}^{out}(t) = \beta_2(t) \cdot F_{inc,t}^{in}(t) \quad (44)$$

$$F_{inc,E}^{out}(t) = \beta_3(t) \cdot F_{inc,t}^{in}(t) \quad (45)$$

$F_{inc,t}^{out}$  is the total outflow of substances from incineration plants,  $F_{inc,B}^{out}$  is the outflow of substances from incineration plants in bottom ash,  $F_{inc,F}^{out}$  is the outflow of substances from incineration plants in fly ash and  $F_{inc,E}^{out}$  is the emissions of substances from incineration plants.

### ***Stock of substances in incineration processes***

The incineration of applications containing the substance in question is one option for the waste management of substances. The change of the magnitude of the stock over time is assumed to be zero as given by Eq. 46. Therefore, the inflow of substances into incineration plants is equal to the outflow of substances from these plants.

$$\frac{dS_{inc}(t)}{dt} = 0 = F_{inc,t}^{in}(t) - F_{inc,t}^{out}(t) \quad (46)$$

where  $F_{inc,t}^{in}(t)$  is the total inflow of the substance into incineration plants from different sources at time  $t$  and  $F_{inc,t}^{out}(t)$  is the total outflow from incineration plants at time  $t$ .

### **3.2.5.4 Landfilling**

#### ***The inflow of substances into landfill sites***

Substances flowing into landfill sites originate from different sources in the economic subsystem: the stock-in-use, recycling and production processes, and the consumption of non-intentional applications of substances.

The inflow of substances into landfill sites from the stock-in-use is estimated in combination with the flow of substances to be incinerated. They are jointly estimated as the difference between the total discarded waste stream from the stock-in-use and the flow collected for recycling, as given by Eq. 31. The inflow of substances into landfill sites from discarded products is estimated as a fraction of the total uncollected flow of each product, as given by Eq. 47.

$$F_{land,DC,i}^{in}(t) = (1 - \alpha_{1,i}(t)) \cdot F_{inc,land,i}^{in}(t) \quad (47)$$

where  $F_{land,DC,i}^{in}$  is the inflow of the substance into landfill sites from the discarded product  $i$  and  $F_{inc,land,i}^{in}$  is the combined inflow of the substance into incineration plants and landfill sites from the discarded product  $i$ .

The total inflow of substances into landfill sites is the inflow of substances from discarded products and from other sources, as given by Eq. 48.

$$F_{land,t}^{in}(t) = \sum_{i=1}^n F_{land,DC,i}^{in}(t) + F_{land,others}^{in}(t) \quad (48)$$

where  $F_{land,others}^{in}$  is the inflow of substances into landfill sites from sources other than discarded products.

Other inflows into landfill sites, including inflow from sewage sludge and from incineration residues can be estimated as model relations.

#### ***The outflow of substances from landfill sites***

The outflow of substances from landfill sites is the amount of these substances that leach into the soil and ground water. The leaching outflow is estimated as a fraction of the stock of substances in landfill sites using a similar equation to Eq. 13.

### ***The stock of substances in landfill sites***

The landfilling of applications containing the substance in question is one option in substance waste management. In this phase, the change of the magnitude of the stock over time is calculated as the difference between the inflow of substances from different sources in the economic subsystem and the outflow of these substances to environmental media (soil and ground water), as given by Eq. 49.

$$\frac{dS_{land}(t)}{dt} = F_{land,t}^{in}(t) - F_{land,t}^{out}(t) \quad (49)$$

where  $F_{land,t}^{in}(t)$  is the total inflow of the substance into landfill sites from different sources at time  $t$  and  $F_{land,t}^{out}(t)$  is the total outflow from landfill sites at time  $t$ .

### **3.2.5.5 Sewage treatment**

Sewage treatment is connected to several substance flows. Its inflows come from emissions during use, from the consumption of food and animal products and from industrial processes, notably the production of other heavy metals. Its outflows are effluent and sewage sludge. Part of the inflow of a substance will end up in sewage sludge and the remainder will end up in the effluent. The sludge can be distributed over soil (used as a fertilizer or soil improvement material), incinerated, sent to, landfill and other destinations.

#### ***Inflow of substances into sewage treatment***

The input of the substance into sewage treatment plants originates from emissions of the substance during the use phase, production processes, the consumption of food and animal products and other sources, as given by Eq. 50.

$$F_{ST}^{in}(t) = F_{CE,ST}^{out}(t) + F_{PP,ST}^{out}(t) + F_{CFA,ST}^{out}(t) + F_{other,ST}^{out}(t) \quad (50)$$

Where  $F_{ST}^{in}(t)$  is the inflow of the substance into sewage treatment plants at time  $t$ ,  $F_{CE,ST}^{out}(t)$  is the flow of the substance originating from emissions during the use phase at time  $t$ ,  $F_{PP,ST}^{out}(t)$  is the flow of the substance originating from production processes, and  $F_{CFA,ST}^{out}(t)$  is the flow of the substance originating from the consumption of food and animal products at time  $t$ .

The inputs of the substance to sewage treatment plants from different sources (consumption, production) are estimated as model relations in the substance use phase.

The input of the substance from the consumption of food and animal products is estimated from the amount of the substance taken by food and fodder from agricultural soil. The uptake of the substance by food and fodder is estimated as a fraction of the substance stock within agricultural soil.

#### ***Outflow of the substances from sewage treatment***

The distribution of the substance between sewage sludge and effluent is mainly determined by the efficiency of the processes and the input volume of the substance.

$$F_{ST,SS}^{out}(t) = \alpha_1 \cdot F_{ST}^{in}(t) \quad (51)$$

$$F_{ST,W}^{out}(t) = F_{ST}^{in}(t) - F_{ST,SS}^{out}(t) \quad (52)$$

where  $F_{ST,SS}^{out}(t)$  is the outflow of the substance from sewage treatment processes with sewage sludge at time  $t$ ,  $F_{ST,W}^{out}(t)$  is the outflow of the substance from sewage treatment processes with water at time  $t$ , and  $\alpha_1$  is the efficiency of the processes.

### ***Sewage sludge***

Sewage sludge is disposed of in different manners. Part is used as a soil improver, part is incinerated and the remainder is landfilled. The future development of disposal routes for sewage sludge can be estimated either by the general equation (Eq. 1) or by using different scenarios (assuming that the most recent values for different disposal routes will remain valid in the future).

$$F^{out}_{SS,S}(t) = \alpha_1 \cdot F^{out}_{ST,SS}(t) \quad (53)$$

$$F^{out}_{SS,INC}(t) = \alpha_2 \cdot F^{out}_{ST,SS}(t) \quad (54)$$

$$F^{out}_{SS,L}(t) = F^{out}_{ST,SS}(t) - F^{out}_{SS,S}(t) - F^{out}_{SS,INC}(t) \quad (55)$$

where  $F^{out}_{SS,S}(t)$  is the flow of the substance in sewage sludge applied to soil, where  $F^{out}_{SS,INC}(t)$  is the flow of the substance with incinerated sewage sludge, and  $F^{out}_{SS,L}(t)$  is the flow of the substance with landfilled sewage sludge.

### **3.2.6 Additional issues related to non-intentional use**

In addition to the intentional use of substances, they also exist as contaminants in applications. This presence is either due to the natural occurrence of substances in ores, such as the presence of lead in phosphate fertilizers, or in fossil fuels, or is due to anthropogenic sources, such as the presence of lead in sewage sludge, incineration and recycling residues.

For these non-intentional applications, the inflows into the economic subsystem are not related to the substance itself but rather to the application in which the substance occurs. In this case each application has to be modelled separately. For some applications there are well developed models and/or scenarios, which can be used directly. In other cases, however, a new model has to be made on the basis of related explanatory variables.

The non-intentional flows of a certain substance in the economic and environmental subsystems are partly related to the waste streams of intentional applications of the substance itself and partly to applications of mixed primary resources.

#### **3.2.6.1 Mixed primary resources**

The inflow of a certain substance through mixed primary resources (coal, oil, other metals ores, phosphate ores, etc.) is determined by the demand for these resources and the proportion of the substance that they contain. Demand for these resources is mainly determined by the demand for final output from the processes in which they are used (e.g. electricity, metals, fertilizer).

In the model a general function (Eq. 56) is used to describe past developments in the demand for the final output from the processes (electricity, oil, heavy metals, and phosphate fertilizers). The same function is used for the future with an assumption on the future development in the explanatory variables.

$$Y(t) = \beta_0 + \sum_{i=1}^n \beta_i X_i(t) + \varepsilon(t) \quad (56)$$

$Y(t)$  is the demand for the final output from the processes at time  $t$ ,  $X_i$ 's are the socio-economic variables at time  $(t)$ ,  $\beta$ 's are the model parameters and  $\varepsilon(t)$  is the model error.

An alternative approach, especially relevant when insufficient data are available or a discontinuity is expected, is the use of scenarios (Image team, 2001).



The input of the substance is modelled based upon the amount of the substance per unit of final output (e.g. per ton of produced metal, kwh electricity, or ton of phosphate fertilizers used) as given by Eq. 57.

$$F_{S,Y}^{in}(t) = Y(t) \cdot S_x \quad (57)$$

Where  $F_{S,Y}^{in}(t)$  is the inflow of the substance at time t, and S is the amount of the substance

### 3.2.6.2 Reusing waste materials

The non-intentional inflows of a certain substance into the economy through intentional applications are due to emissions during the use phase, which partly end up in sewage sludge, and the processing of their waste streams. These flows are determined by the demand for the substance in intentional applications, their life span, the emission factors and the waste management of discarded products.

The input of the substance through sewage sludge originates from sewage treatment plants and the input of substances into sewage treatment plants is discussed in section 3.2.5.5.

The input of the substance into incineration plants originates from the waste stream of the products containing the substance which have been discarded from the stock-in-use, together with that part of the produced sewage sludge which is incinerated, as given by Eq. 58.

$$F_{inc}^{in}(t) = \sum_{i=1}^n F_{inc,DC,i}^{in}(t) + F_{inc,SS}^{in}(t) \quad (58)$$

The input from sewage sludge is estimated as a fraction of the substance in the sewage sludge. Other options for sewage sludge include disposal in landfill sites, application to the soil, and others as discussed in section 3.2.5.5.

The input from the discarded outflow from the stock-in-use is estimated from an assumption about the distribution between incineration, landfill and recycling as discussed in section 3.2.5.3.

### 3.2.6.3 Output of substances from different processes

Outflows of the substance from the production processes of final outputs (oil, electricity, other heavy metals) and the incineration processes are mainly determined by technical factors. These outflows are modelled as a fraction of the input, as given by Eq. 59. Mass balance is enforced by modelling one flow per process as a balancing item.

$$F_{S,x}^{out}(t) = \alpha_x(t) \cdot F_{S,Y}^{in}(t) \quad (59)$$

Where  $F_{S,x}^{out}(t)$  is the outflow of the substance to a specific destination at time t,  $\alpha_x(t)$  represents the emissions factor, the division of the substance between fly and bottom ashes, and the different disposal routes of sewage sludge at time t.

The emission factors are mainly determined by technological development. They are assumed either to be constant or to change over time. The emission data are fitted to a linear function similar to that given by Eq. 56, using time as proxy of technological development and other time-related variables, or they are fitted to an exponential function as given by Eq. 60.

$$\alpha_x(t) = \beta_0 \cdot e^{\beta_1 \cdot t} \quad (60)$$

The division of the substance to bottom ash and fly ash during incineration processes and electricity production is determined by technical factors and given in different sources (Hasselriis and Licata, 1996, Sandelin et al. 1999 & Sandelin et al. 2001).

The disposal routes of sewage sludge are mainly determined by policy aspects. These can be assumed to be constant and use the most recent values, or can be assumed to change over time, in which case they can be modelled based on Eq. 56. Time can be used as a proxy of the policy aspects and other time-related variables.

### 3.2.6.3 The agricultural cycle

Stock building of substances takes place in agricultural soil. Figure 6 shows the flows connected to the stock of substances in agricultural soil.

#### *Inflow of substances into the agricultural soil stock*

The inflow of a substance into agricultural soil originates from different sources, including the application of materials to agricultural soil (e.g. fertilizers, sewage sludge and manure) and deposition from the air.

$$F_S^{in}(t) = F_{AD,S}^{out}(t) + F_{F,S}^{in}(t) + F_{SS,S}^{out}(t) + F_{M,S}^{in}(t) \quad (61)$$

where  $F_{AD,S}^{out}(t)$  is the deposited flow from the air  $F_{F,S}^{in}(t)$  is the flow of fertilizers,  $F_{SS,S}^{out}(t)$  is the flow from sewage sludge and  $F_{M,S}^{in}(t)$  is flow of manure.

#### *Outflow of substances from agricultural soil stock*

The outflow of a substance from agricultural soil is the amount of the substance taken up by plants (food and fodder crops) plus the amount of leaching of the substance to the ground water. The flow of a substance taken up by plants further contributes to the substance stock in soil through loops within the subsystem, related particularly to animal production (manure) and food products (sewage sludge).

$$F_{S,FOOD}^{out}(t) = \alpha_1 \cdot S_S(t) \quad (62)$$

$$F_{S,FODDER}^{out}(t) = \alpha_2 \cdot S_S(t) \quad (63)$$

$$F_{S,L}^{out}(t) = \alpha_3 \cdot S_S(t) \quad (64)$$

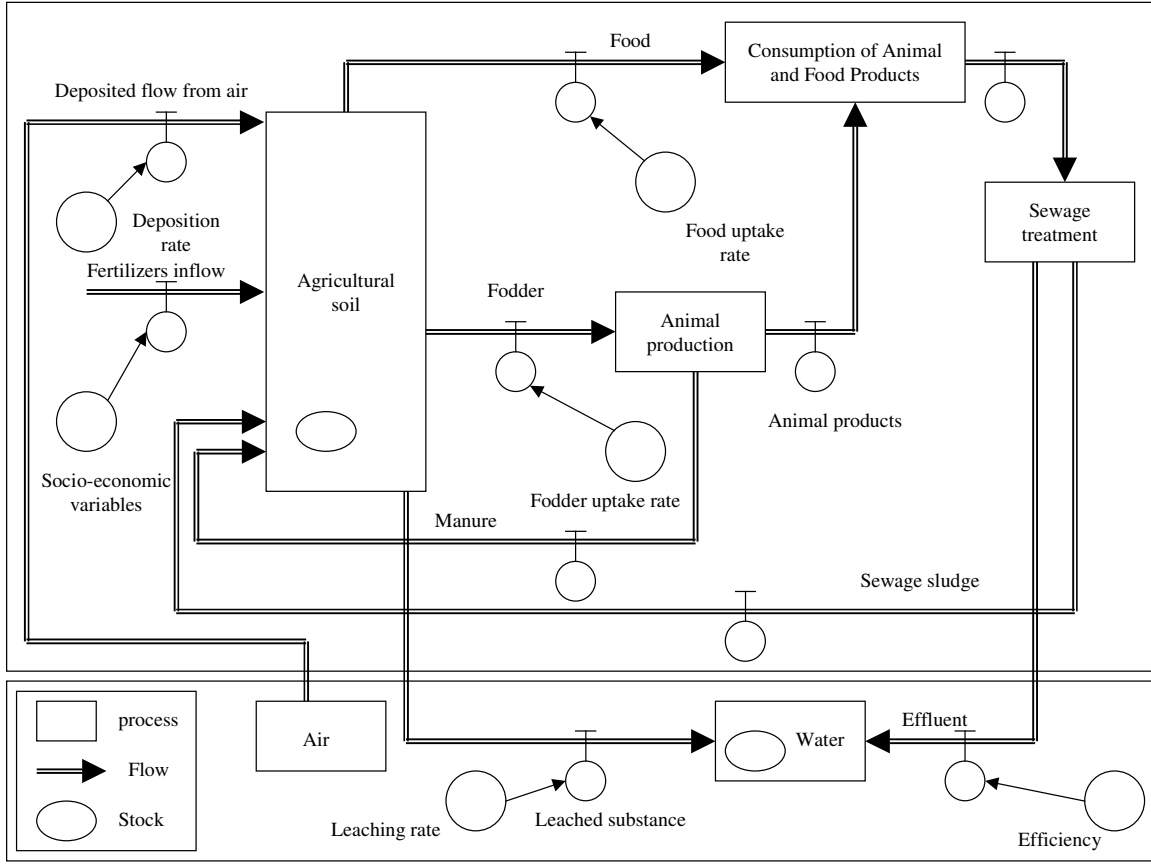
where  $F_{S,FOOD}^{out}(t)$  is the uptake outflow of the substance from agricultural soil to food,  $F_{S,FODDER}^{out}(t)$  is the uptake outflow of the substance from agricultural soil to fodder,  $F_{S,L}^{out}(t)$  is the leaching outflow of the substance from agricultural soil to water.  $\alpha_1$  is the uptake rate for food,  $\alpha_2$  is the uptake rate for fodder, and  $\alpha_3$  is the leaching rate.

#### *Stock of substances in agricultural soil*

The change of the magnitude of the substance stock in the soil over time is determined by the inflow of the substance into the soil through different sources and the outflow of the substance from the soil, given by Eq. 65.

$$\frac{dS_S}{dt} = F_S^{in}(t) - F_S^{out}(t) \quad (65)$$

where  $F_S^{in}(t)$  is the inflow into the stock at time t,  $F_S^{out}(t)$  is the outflow from the stock at time t



**Fig. 6:** The flows connected to the stock of substances in agricultural soil

### ***Animal production***

The inflow of a substance into animal production is the result of the output of the substance from the soil in the form of fodder. The outflow of a substance from animal production is the amount of the substance in manure plus the amount which goes to consumption of food and animal products (Eq. 66). The total outflow from animal production is equal to the total inflow into animal production.

$$F_{An}^{out}(t) = F_{CFA,An}^{in}(t) + F_{M,S}^{in}(t) \quad (66)$$

$$F_{CFA,An}^{in}(t) = \alpha \cdot F_{An}^{out}(t) = \alpha \cdot F_{An}^{in}(t) = \alpha \cdot F_{S,FODDER}^{out}(t) \quad (67)$$

$$F_{M,S}^{in}(t) = (1 - \alpha) \cdot F_{An}^{out}(t) = (1 - \alpha) \cdot F_{An}^{in}(t) = (1 - \alpha) \cdot F_{S,FODDER}^{out}(t) \quad (68)$$

where  $F_{An}^{out}(t)$  is the outflow of the substance from animal production,  $F_{CFA,An}^{in}(t)$  is the inflow of the substance into the consumption of food and animal products from animal production, and  $F_{M,S}^{in}(t)$  is the flow of manure from animal production.

### ***Consumption of food and animal production***

The inflows of a substance into the consumption of food and animal products, as given by Eq. 69, are the flows of the substance through food products, as given by Eq. 62 and the flows of the substance from

animal production, as given by Eq. 66. The outflow from food and animal production enters sewage treatment, as given by Eq. 70, and is equal to the total inflow.

$$F_{CFA}^{in}(t) = F_{S,FOOD}^{out}(t) + F_{CFA,An}^{in}(t) \quad (69)$$

$$F_{CFA}^{out}(t) = F_{CFA,ST}^{out}(t) \quad (70)$$

where  $F_{CFA,ST}^{out}(t)$  is the outflow of the substance from the consumption of food and animal products to sewage treatment.

### 3.2.7 Modelling imports and exports

Substance flow analysis can be carried out at different levels; international, national, and local. If the modelled system is small (national or local), the import and export of products, scrap and the refined substance should be taken into account. Figure 7 shows the processes, intentional flows and stocks in national or local economic subsystems.

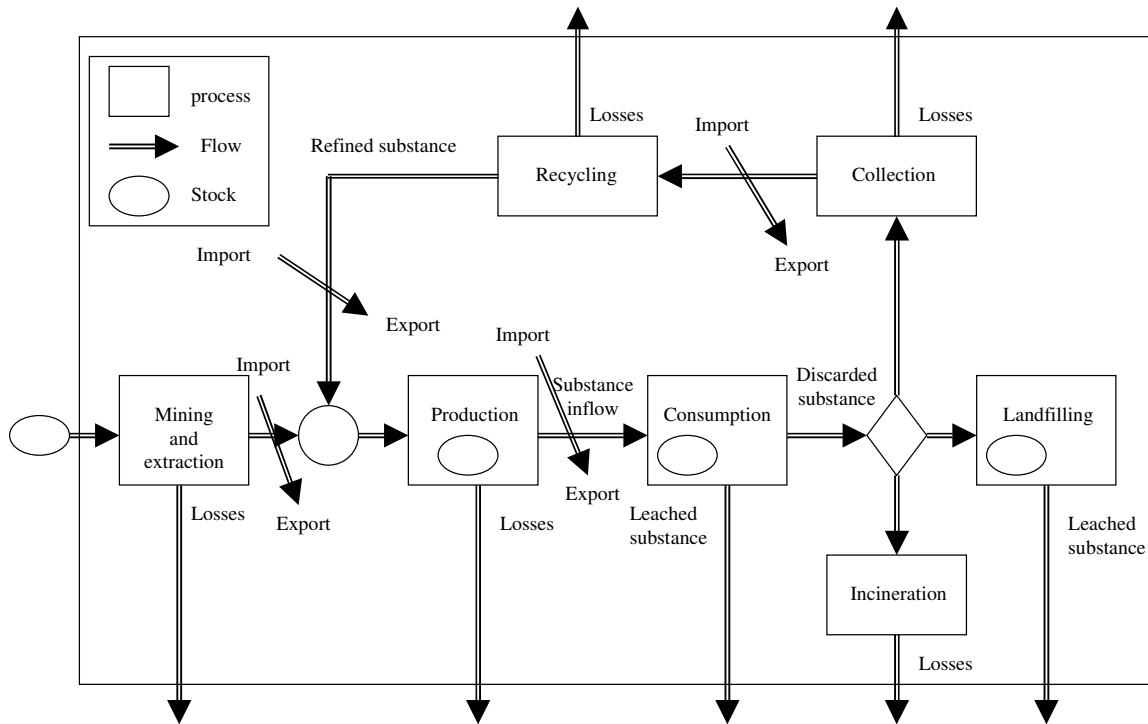


Fig. 7: The main flows, stocks and processes in a national or local economic subsystem.

#### 3.2.7.1 Imports and exports of products

The inflow of a substance  $F_{C,i}^{in}$  into the stock-in-use in a country is equal to the amount of the substance in the products produced in the country  $F_{PP,i,P}^{out}$  plus imported products minus exported products, as given by Eq. 71.

$$F_{C,i}^{in}(t) = F_{PP,i,P}^{out}(t) + import(t) - export(t) \quad (71)$$

The import and export of products is estimated as the difference between the products produced in a country and the inflow of products into the consumption phase from Eq. 71 (i.e. as a balancing item).

between the production and consumption phases). It is difficult to separate the estimated value for imports and exports, and therefore the estimated value is kept as one variable, net imports. Eq. 2 gives the inflow of the substance into the use phase. In the model, a general function similar to Eq. 1 is used to describe the outflow of the substance within products  $F_{PP,i,P}^{out}(t)$  based on the past trend data.

The production of a certain product in a specific country is determined by the global demand for products and the competition in the world market, which are affected by energy and labour costs, indicated by GDP/C, and the cost of disposing of any residual materials. The substance content of a product is determined by substitution and technical developments.

### 3.2.7.2 Imports and exports of obsolete products

The import and export of obsolete products are estimated as the difference between the products collected in a country and the inflow of obsolete products into recycling processes from Eq. 72 (i.e. as a balancing item between the collection and recycling phases). It is difficult to estimate the value of imports and exports separately, and therefore the estimated value is kept as one variable, net imports.

$$F_R^{in}(t) = F_{SC,R}^{out}(t) + import(t) - export(t) \quad (72)$$

The outflow of obsolete products to recycling processes is estimated in Eq. 32. The inflow of obsolete products into recycling processes is estimated as a balancing item for recycling processes. In this case, it is not possible to estimate the outflow from recycling processes (as given by Eqs. 34 and 35). Instead, the usable secondary material (one of the outflows of recycling) can be estimated on the basis of explanatory variables. A general function similar to Eq. 1 is used to describe the outflow  $F_{R,R}^{out}$ , which is based on past trend data.

The most influential factors in this respect are: the costs of sorting and transformation, of disposing of any residual material, of energy and labour indicated by GDP/C, together with global demand for the material, and the price of secondary material compared to that of primary material.

### 3.2.7.3 Import and export of primary and secondary refined substances

The inflow of a substance  $F_{PP}^{in}$  into the production processes within a country is the amount of the substance (primary and secondary) produced in the country plus the imported amount of the substance minus the exported amount as given by Eq. 73.

$$F_{PP}^{in}(t) = F_{R,R}^{out}(t) + F_{R,P}^{out}(t) + import(t) - export(t) \quad (73)$$

where  $F_{R,R}^{out}(t)$  is secondary refined substance in the country at time t, which is known from recycling processes,  $F_{R,P}^{out}(t)$  is the primary refined substance in the country at time t.

The import and export of primary and secondary substances can be estimated as the difference between the primary and secondary refined substance produced in a country and the inflow of substances (primary and secondary) into the production processes of the substance-containing applications (i.e. as a balancing item between the recycling and production phases). In most cases, it is possible to estimate the production of refined substances (primary and secondary) in the future. Data about the inflow of these substances into the production processes of their applications is generally not directly available, but it is possible to estimate the inflows as described in section 3.2.4. By estimating the inflow directly from Eq. 24, the value of imports minus exports can be estimated from Eq. 73. As it is difficult to estimate the values of the imports and exports separately, the estimated value is presented as one variable, net imports.

### 3.3 Environmental subsystem

Substance flows and stocks in different environmental compartments originate from the substances used in economic activities (production, consumption, and waste management), whether these activities are related to the intentional use or non-intentional use of a substance. Figure 8 shows the environmental stocks and flows. The environmental subsystem includes several components; air, water, non-agricultural soil, sediment, ground water and sea water. In this study air, fresh water and soil are distinguished as separate components in the model. The environmental subsystem includes two stocks; stocks in non-agricultural soil and resource stocks. The substance flows and stocks in the different environmental components are interconnected, with flows from one to another. These flows and stocks are only partially included in the model – more detailed modelling of these flows and stocks can be done through multi-media fate modelling (Heijungs, 2000).

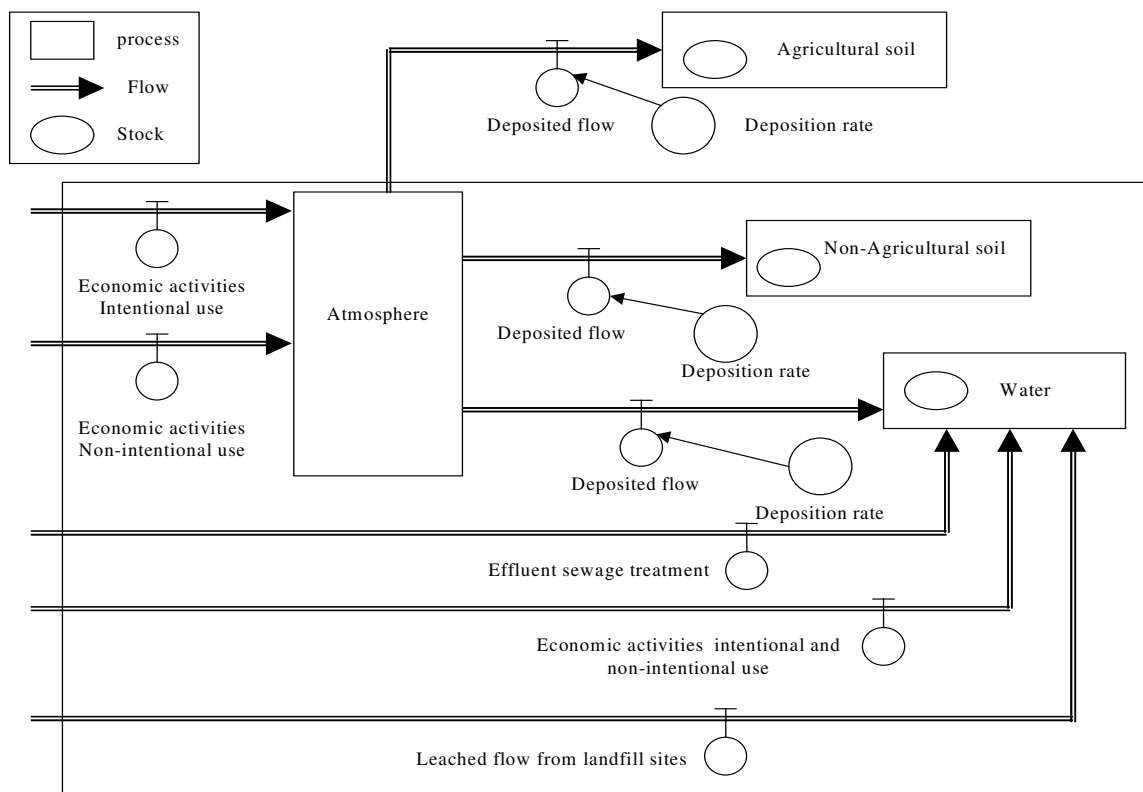


Fig. 8: Stocks and flows in the environmental subsystem.

#### 3.3.1 Air

##### *Inflow of substances into air*

The inflow of a substance into the air originates from different sources, some of which are related to the intentional use of the substance and others to non-intentional use.

$$F_A^{in}(t) = \sum F_{PP,i,A}^{out}(t) + F_{inc,A}^{out}(t) + F_{R,A}^{out}(t) + F_{C,E}^{out}(t) + F_{NIU,A}^{out}(t) \quad (74)$$

where  $F_{PP,i,A}^{out}$  is emissions from the production of different applications,  $F_{inc,A}^{out}$  is emissions from the incineration process,  $F_{R,A}^{out}$  is emissions from recycling processes,  $F_{C,E}^{out}$  is emissions from use of different applications,  $F_{NIU,A}^{out}$  is emissions from non-intentional use.

### ***Outflow of substances from the air***

The outflow of a certain substance from the air, which is equal to the total inflow, is the amount of the substance deposited in water, soil (agricultural and non-agricultural) and outside the region (trans-boundary flow).

$$F_A^{out}(t) = \sum_{i=1}^n F_{A,i}^{out}(t) \quad (75)$$

$$F_{A,DS}^{out}(t) = \alpha_1 \cdot F_A^{in}(t) \quad (76)$$

$$F_{A,DW}^{out}(t) = \alpha_2 \cdot F_A^{in}(t) \quad (77)$$

$$F_{A,TF}^{out}(t) = F_A^{in}(t) - F_{A,DS}^{out}(t) - F_{A,DW}^{out}(t) \quad (78)$$

where  $F_A^{out}$  is the total outflow from of the substance from the air,  $F_{A,DS}^{out}$  is the deposited flow of the substance in the soil,  $F_{A,DW}^{out}$  is the deposited flow of the substance in water, and  $F_{A,TF}^{out}$  is the deposited flow of the substance outside the modelled system

### **3.3.2 Water**

#### ***Inflow of substances into water***

The inflow of a certain substance into water originates from different sources, some related to the intentional use of the substance and others to its non-intentional use.

$$F_W^{in}(t) = \sum F_{PP,i,W}^{out}(t) + F_{R,W}^{out}(t) + F_{NIU,W}^{out}(t) + F_{A,DW}^{out}(t) + F_{land,W}^{out}(t), F_{ST,W}^{out}(t) \quad (79)$$

$F_{PP,i,W}^{out}$  is emissions from the production of different applications,  $F_{R,W}^{out}$  is emissions from recycling processes,  $F_{NIU,W}^{out}$  is emissions from non-intentional use,  $F_{A,DW}^{out}$  is deposition from the air,  $F_{land,W}^{out}$  is leaching from landfill sites,  $F_{ST,W}^{out}$  is effluent from sewage.

### **3.3.3 Non-agricultural soil**

Soil is divided into two component parts, agricultural soil, which is treated in the economic subsystem and non-agricultural soil. The change of the magnitude of the substance stock in non-agricultural soil over time is determined by the inflow of the substance into the soil from different sources and the outflow of the substance from it as given by Eq. 80. The model treats non-agricultural soil as a sink, from which there is no outflow from stock.

$$\frac{dS_s}{dt} = F_s^{in}(t) - F_s^{out}(t) \quad (80)$$

where  $F_s^{in}(t)$  is the inflow into the stock at time t,  $F_s^{out}(t)$  is the outflow from the stock at time t and equal to zero in the model.

#### ***Inflow of substances into non-agricultural soil***

The inflow of a substance to non-agricultural soil originates from different sources, some related to the intentional use of the substance and others to its non-intentional use.

$$F_S^{in}(t) = \sum F_{C,E}^{out}(t) + F_{NIU,S}^{out}(t) + F_{A,DS}^{out}(t) + F_{land,S}^{out}(t) \quad (81)$$

where  $F_{C,E}^{out}$  is emissions from the use of different applications,  $F_{NIU,A}^{out}$  is emissions from non-intentional use,  $F_{A,DS}^{out}$  is deposition from the air,  $F_{land,S}^{out}$  is leaching from landfill sites.

### 3.3.4 Resource stock

The change in the stock of a substance resource in ores is determined by demand for the substance from primary resources and consequently the amount being extracted from the ores and the addition to the stock, which is determined by the initial resource stock taken in the model. Two types of resources can be classified; identified resources and current reserves (USGS and USBM, 1980). Current reserves include all substance resources that are economic to extract at the current market price using existing technology. Identified resources include economic, marginally economic and sub-economic resources.

If the identified resources are used as the measure of the resource, this in principle gives a fixed amount and additions to the stock are assumed to be zero. If, however, the economic current reserve is taken as the measure, the resource stock can change with changes in techniques or prices. In this case, the addition to the stock will be the part of the identified resources, which is currently not economic or technically feasible to extract.

$$\frac{dS_{Res}(t)}{dt} = F_{Res}^{in}(t) - F_{Res}^{out}(t) = F_{Res}^{in}(t) - F_P^{in}(t) \quad (82)$$

where  $F_{Res(t)}^{in}$  is the addition to the stock of resources at time  $t$ ,  $F_{Res(t)}^{out}$  is the outflow of the substance from the stock of resources at time  $t$ , and  $F_{P(t)}^{in}$  is the inflow of the substance into primary production processes at time  $t$ .

## 3.4 Methods used in the evaluation of model variables and parameters

Several mathematical and statistical methods are used in the evaluation of some of the model's variables and parameters, such as the inflow of substances into the stock-in-use, the substance content in products, emission factors, and product life spans. These methods are briefly described below.

### 3.4.1 Evaluating the equation used in the inflow of substances into the stock-in-use

#### *Regression analysis*

Regression analysis is used in several scientific fields as a statistical tool to analyze the relation between variables. For example, it has been used to describe the demand for electricity, metals and other commodities as a function of socio-economic variables such as GDP, population, price and other specific variables for each commodity (Burney, 1995; Ranjan and Jain, 1999; Mohamed and Bodger, 2005; Roberts, 1996; Moore et al. 1996).

Regression analysis is used in the analysis to establish the relative importance of the independent variables on the shape of the inflow curve over time. It identifies the most significant variables, which contribute most to the shape of the inflow curve. It also examines the combined effect of significant variables. The fitting algorithm that determines the regression parameters ( $\beta^s$ ) uses the ordinary least square (OLS) criterion (Gijbels and Rousson, 2001).

The adequacy of the regression model and the significance of the variables can be described in statistical terms. The adjusted coefficient of determination ( $R^2_{adj}$ ) and F-statistics can be used to determine the overall goodness of the regression model. T-statistics can be used to evaluate the significance of the individual variables in the model.

$R^2$  is a measure of how much of the variance in the dependent variables is explained by the independent variables in the regression model. Large values of  $R^2$  indicate better agreement between the model and the data. However,  $R^2$  will always increase as more variables are added to the model. As an alternative,  $R^2_{adj}$



can be used when more than one variable is combined in the model and this takes into account the number of independent variables. F-statistics indicate whether adding another variable to the regression model significantly improves the quality of the fit. T-statistics indicate whether or not each regression coefficient is significantly different from zero. For F-statistics and T-statistics, the critical value indicating the significance of the model, or its individual variables, at different probability levels can be found in statistical books.

### ***Learning curve concept***

The learning or experience curve concept is an analytical tool that can be used to provide a quantitative, mostly exponential, relation between a certain input to a process (Y) and a cumulative output (X) (Eq. 83). The parameter (-r) is referred to as the experience index and is defined by the progress ratio (F) and the learning rate (L). Eq. 84 and Eq. 85 give the progress ratio and the learning rate.

$$Y = a \cdot X^{-r} \quad (83)$$

$$F = 2^{-r} \quad (84)$$

$$L = 1 - 2^{-r} \quad (85)$$

where a in Eq. 83 is the value of Y for the first unit produced

The progress ratio (F) shows how an input Y will be reduced when the cumulative output is doubled. For instance, when F= 90% and L=10%, the input Y will be reduced to 90% of its previous level each time the cumulative output is doubled. In general, the progress ratio may increase over time for some technologies (Junginger et al., 2003, and Karaoz and Albeni, 2005).

The learning curve concept is used to model the relation between cost and cumulative production (Junginger et al 2005, Tsuchia and Kobayashi, 2004) and the relation between the energy consumption and cumulative production (Ruth, 1998, Ayres et al., 2003, and Ramirez and Worrell, 2006).

In the present model, the learning curve concept is used to model the possible reduction in the substance content of a product or material over time, the possible reduction in energy use in mining, smelting and refining processes, and possible reductions in ore grade over time.

### **3.4.2 Evaluating the distributions of the discarded outflow from the stock-in-use**

In most studies, the life span of products is assumed to be a fixed number, an average value of several randomly occurring life spans. In reality however, products may have different life spans, depending on their technical specifications and the way they are used by consumers. To overcome the uncertainty associated with the assumed average life span, statistical distributions are performed to mathematically describe or model a certain life span behaviour. The probability density function (p.d.f.) is a mathematical function that describes this distribution. Common types of distribution are normal, lognormal and Weibull distributions. The Weibull distribution, which is also called lifetime distribution, was formulated by Professor Wallodi Weibull and is commonly used for analyzing life span data. This model uses the Weibull distribution, as it has been shown experimentally that it provides a good fit to the life span of many types of products (Melo,1999). The Weibull distribution is characterized by three parameters, the shape parameter  $\beta$ , which defines the shape of the curve, the scale parameter  $\alpha$ , which defines where the bulk of the distribution lies and the location parameter a, which defines the location of the distribution in time. The mathematical formulas for the Weibull distribution are given below.

Probability density function (p.d.f.) of the Weibull distribution is given by

$$p.d.f = \alpha \beta^{-\alpha} (t - a)^{\alpha-1} \exp\left[-((t - a)/\beta)^{\alpha}\right] \quad (86)$$

$$P_t = \int_t^{t+1} f(x)dx \quad (87)$$

$$f(x) \Rightarrow p.d.f \quad (88)$$

The probability that a product has a life span of  $t$  years is given by

$$P_t = \exp\left[-((t-a)/\beta)^\alpha\right] - \exp\left[-((t+1-a)/\beta)^\alpha\right] \quad a \leq t < b \quad (89)$$

To determine the value of the parameters  $\alpha$  and  $\beta$  the following equations can be used (Melo, 1999)

$$\gamma = 1 - \exp\left[-((b-a)/\beta)^\alpha\right] = 0.997 \quad (90)$$

$$\alpha \ln\left(\frac{b-a}{m-a}\right) + \ln\left(\frac{\alpha-1}{\alpha}\right) - \theta = 0 \quad (91)$$

where  $a$  is the minimum life span,  $b$  is the maximum life span and  $m$  is the most likely life span.

$$a + \beta\left(\frac{\alpha-1}{\alpha}\right)^{1/\alpha} = m \quad \alpha \geq 1 \quad (92)$$

With the knowledge of parameters  $\alpha$  and  $\beta$ , the mean and the variance of the distribution can be determined.

$$\mu = a + \frac{\beta}{\alpha} \Gamma\left(\frac{1}{\alpha}\right) \quad (93)$$

$$\sigma^2 = \frac{\beta^2}{\alpha} \left\{ 2\Gamma\left(\frac{2}{\alpha}\right) - \frac{1}{\alpha} \left[ \Gamma\left(\frac{1}{\alpha}\right) \right]^2 \right\} \quad (94)$$

with  $\Gamma(x)$  as the Gamma function

$$\Gamma = \int_0^\infty t^{x-1} e^{-t} dt \quad (95)$$

### 3.4.3 Evaluating the emission factors of processes

The emission factors for some processes are taken directly from the literature. For others, however, the emission factors have been evaluated in different manners. For example, the emission factor for producing catalytic converters (CC) is estimated using several parameters: the number of vehicles with CC, the average driving distance per vehicle, the emissions per km, and the platinum loading per CC. The platinum emission factor was estimated for three countries, and the average was used in the model.

### 3.4.4 Solving the differential equations

The differential equation given by Eq. 17 can be solved numerically by stepwise integration (Euler's method)

$$S(t + \Delta t) \approx S(t) + \frac{dS}{dt} \Delta t \quad (96)$$

$$S(t + \Delta t) \approx S(t) + [F^{in}(t) - F^{out}(t)] * \Delta t \quad (97)$$

By knowing the initial value of the stock at time  $t$  and the inflow, it is possible to calculate the stock as given by Eq. 98.

$$S_c(t + 1) = S_c(t) + F_c^{in}(t) - F_c^{out}(t) \quad (98)$$

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## **Chapter 4    Dynamic Stock Modelling: A Method for the Identification and Estimation of Future Waste Streams and Emissions Based on Past Production and Product Stock Characteristics \***

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### **Abstract**

Large quantities of products, materials and substances have accumulated in society. This chapter investigates the dynamic behaviour of these societal reservoirs or stocks in order to explore future emissions and waste streams. We argue that the stock dynamics are mainly determined by its inflow and outflow characteristics. The stock's inflow is determined by socio-economic factors, which can be quantified using regression analysis. Two processes determine the stock's outflow: leaching and delay. Leaching occurs during use and can be modelled as a function of the stock's size. Delay is related to the discarding of products after use and can be modelled as a delayed inflow distributed over time. This approach is illustrated by the case of lead as applied in cathode ray tubes in the European Union (EU). By applying this model to other lead applications and combining the results, the dynamic behaviour of the total lead stock in society can be described.

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\* Reprinted from “Elshkaki, A., Van der Voet, E., Van Holderbeke, M., and Timmermans, V. (2005). Energy; 30, 8, 1353-1363”.

## 4.1 Introduction

Extraction, use and discarding of materials causes environmental problems. Some of these problems are related to resource depletion, others to pollution resulting from emissions during the life cycle of these materials. A relatively new field of research, industrial ecology, studies society's metabolism to analyse the causes of these problems and indicate possibilities for a more sustainable management of materials. Substance flow analysis (SFA) is one of the main analytical tools within the industrial ecology research field. SFA is used to describe or analyse the flows of one substance (group) in, out and through a system (Van de Voet, 1996). The system is a physical entity, often representing a geographical area. In most cases, the SFA system is divided into two subsystems: the economic or societal subsystem and the environmental subsystem.

SFA is based on the materials balance principle, which enables different types of analysis. Substance flow accounts can be used to identify major flows and accumulations and, if available for several years, to spot trends. Static SFA models can be used to identify the causes of pollution problems and to assess the effectiveness of measures (Udo de Haes et al. 1997). The main difference between static and dynamic models in SFA lies in the inclusion of stocks in society (Bergback and Lohm, 1997). Stocks of products and materials in use are a major cause of disconnection between the system's inflow and its outflow in one year. Ignoring them may lead to erratic forecasts of future emissions and waste streams. Dynamic SFA models including stocks lead to more accurate prediction of future resource use and waste streams. Considering stocks so far has resulted in a few specific substance stock inventories or models (Boelens and Olsthoorn 1998 and Kleijn and Van der Voet, 1998). This chapter contains an effort to define a general stock model. The dynamics that determine the growth and decline of the stocks of a substance over time are determined by the inflow and outflow of the materials and products that contain it. This chapter will focus on the inflow, which in turn is determined by the demand for the products containing those materials and substances.

Over the last century, the increase of the global population and the GDP per head in developed countries has been accompanied by a rapid increase in material consumption (Bergback and Lohm, 1997). In fact, the overall level of national income, the product composition of income and material composition of product have been used in determining the intensity of use of materials in several studies (Tilton, 1990 and Moor and Tilton, 1996). In this chapter, a likewise approach is adapted to estimate the stock's inflow. The modelling of the stock's outflow is mainly based on physical consideration, especially mass balance.

The next section will outline a methodology for dynamic stock modelling, followed by a description of the cathode ray tube system, and finally a section containing a discussion of the results and some conclusions.

## 4.2 Dynamic stock modelling approach

In the use phase, goods with a life span of more than one year tend to accumulate: they do not flow out again in the same year but remain stored for some time as products-in-use. Such applications stored in the use phase are referred to as stocks. The mechanism determining the stock dynamics can be classified into three levels:

- stocks of products, handled by producers and users (e.g. cathode ray tubes)
- stocks of materials that those products are composed of (e.g. lead oxide) and
- stocks of substances, contained within these materials and hence products (e.g. lead).

Stocks on these three levels have their own characteristics and dynamic behaviour.

The demand for a particular product is determined by significant variables such as its price compared to the price of the closest substitute, and the level of overall economic activities (Tilton, 1990). Moreover, in the course of time technological developments may also affect the demand for a particular product because of the emergence of alternatives. It may also affect the demand for materials due to changes in product design. For example, the developments in lead-acid battery technology led to a reduction of the total weight of a battery from about 19 kg to 16.6 kg over a period of 15 year. Most of the reduction of about 2.5 kg was obtained through reducing the lead content of the battery (ILZSG, 1999).

The dynamic behaviour of the product stock, which is mainly determined by the behaviour of the stock's inflow (purchases of new products) and stock's outflow (discarding of obsolete products) will be described in the following sections.

### 4.2.1 Modelling the product stock inflow

The total inflow into a particular stock of products-in-use is determined by supply and demand, each of these in turn determined by several further variables. Among these are socio-economic variables such as GDP, population, technological developments and welfare, as well as other economic factors such as the presence of alternatives and their relative prices. It is useful to start by making a qualitative model of the system. For example, it must be established whether or not there are any substitutes for the product, and if so, what their specifications are regarding material composition, performance and price. It is also relevant to know whether or not the product at present is subject to rapid change due to technological improvements, and if so, in which direction.

The second step is to quantify the relationship between the inflow of the product and the most influential variables (e.g. population, GDP). Time series data are required for the inflow on the one hand, and the explanatory variables on the other hand.

To establish the relative importance of these variables on the shape of the inflow curve over time, a regression model can be used. Regression analysis indicates the variables that are significant and contribute most to the shape of the inflow curve. It also examines the combined effect of significant variables.

The linear regression model used in this analysis is described by Eq. (1):

$$Y(t) = \beta_0 + \beta_1 \cdot X_1(t) + \beta_2 \cdot X_2(t) + \beta_3 \cdot X_3(t) + \beta_4 \cdot X_4(t) + \beta_5 \cdot X_5(t) + \varepsilon(t) \quad (1)$$

where  $Y$  is the inflow of a particular good, the variables  $X_1, X_2, X_3, X_4$ , and  $X_5$  are indicating the different influential variables, the parameters  $\beta_0, \beta_1, \beta_2, \beta_3, \beta_4$ , and  $\beta_5$  are the regression parameters and  $\varepsilon$  is the model error

The adequacy of the regression model and the significance of the variables can be described in statistical terms such as the adjusted coefficient of determinations ( $R^2_{adj}$ ), t tests and F statistics.

The derived regression model described by Eq. (1) can further be used to estimate the future inflow of goods. Projected values of the influential variables are then required. Such projections are available for GDP and population in different scenario studies (RIVM, 2001).

### 4.2.2 Modelling the product stock outflow

The outflow out of the stocks depends on the mechanisms of delay and leaching. Delay represents the discarding of products and is determined by the life span of the products. Empirical data on the life span is often not available (Kleijn et al. 2000). Either an average life span or a certain life span distribution can be assumed. Possible types of distribution are normal, Weibull, or beta distributions. In this study, the Weibull distribution has been used since it has been shown experimentally that Weibull distribution provides a good fit to the life span of many types of products (Melo, 1999). The outflow from the societal stock due to discarding is given by Eq. (2):

$$F^{out}(t) = F^{in}(t - L) \quad (2)$$

where  $F^{out}(t)$  is the outflow of goods at time  $t$ ,  $F^{in}$  is the inflow of goods, and  $L$  is the life span.

Leaching refers to the emissions of the substance from the products during the use process. The emissions during use can be described as a fraction of the stock. For different applications, an emission rate can be established. For heavy metals for example, there are studies aimed at establishing a leaching coefficient describing the corrosion from surfaces exposed to the environment (Bentum, 1996). The outflow during use is given by Eq. (3).

$$F^{out}(t) = C \cdot S(t) \quad (3)$$

where  $S$  is the size of the stock at time  $t$  and  $C$  is the leaching factor.

Reuse of products indirectly influences the stock's inflow as well as outflow. Reuse can be affected by several factors. Among these are technical and economic factors, which determine mainly the collection rate, and environmental policy aspects. When reuse must be modelled, these factors should be accounted for. In this model, the flow of waste products destined for reuse is modelled as a fraction of the total outflow by discarding as given by Eq. (4). On the material and substance level, recycling also plays a role.

$$R(t) = \alpha \cdot F^{out}(t) \quad (4)$$

where  $R(t)$  is the amount to be reused at time  $t$ ,  $\alpha$  is the reuse rate and  $F^{out}(t)$  is the outflow of discarded goods as calculated by Eq. (2).

### 4.2.3 Modelling the product stock size

The change of the magnitude of the stock over time is the difference between the inflow and the outflow as given by Eq. (5).

$$\frac{dS}{dt} = F^{in}(t) - F^{out}(t) \quad (5)$$

By knowing the initial value of the stock and the inflow of goods, it is possible to calculate the stock as given by Eq. (6) and the future outflow using Eqs. (2) and (3).

$$S(t+1) = S(t) + F^{in}(t) - F^{out}(t) \quad (6)$$

## 4.3 Case study – Lead in cathode ray tubes

Lead was one of the first metals used by humankind, and its use has been extensive throughout history. Its unique properties such as its corrosion resistance, high density and low melting point make it suitable for several applications. A considerable use of lead is its application as a compound in cathode ray tubes (CRTs). A CRT is one of the components of television and computer monitors. Lead is used in CRTs as a protection from harmful radiation. The average weight of one CRT is 13 kg, of which 2 kg is taken up by lead. Figure 1 shows the CRT life cycle. The stock of CRTs is a part of this life cycle: it is accumulated in the “use” phase.

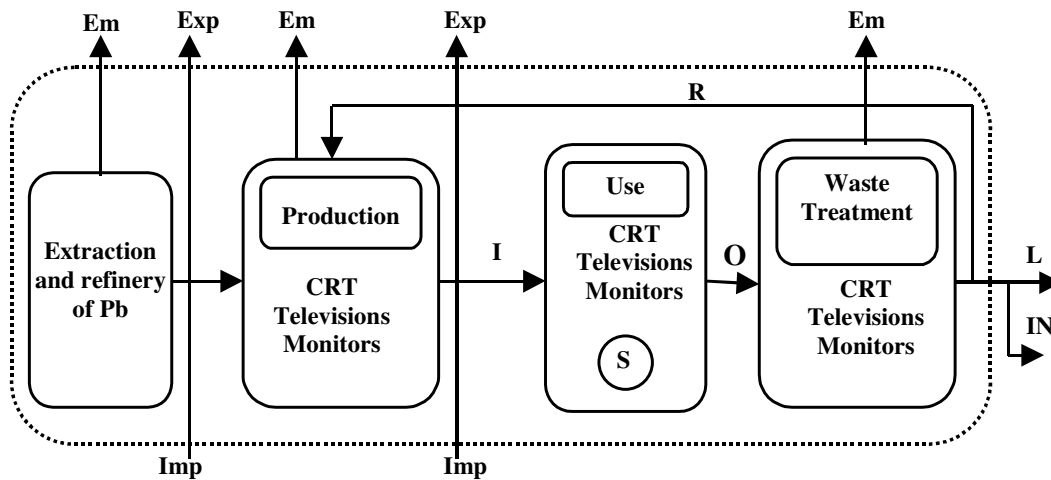


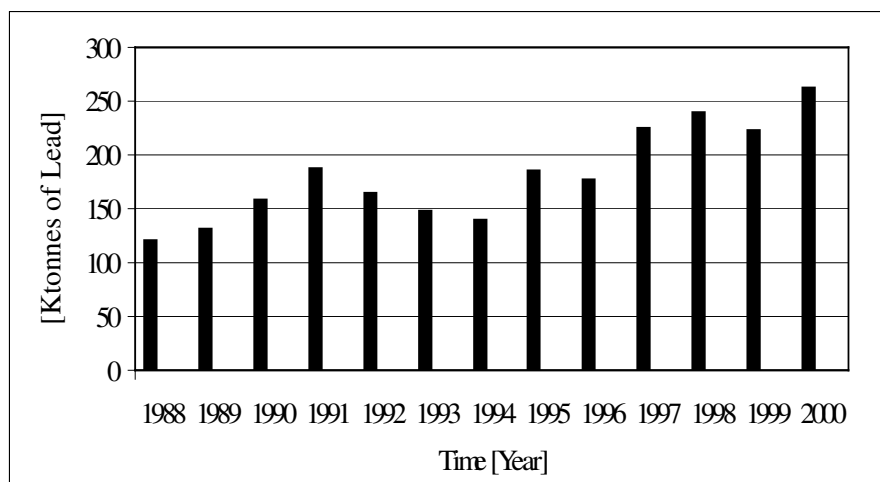
Fig. 1: The CRT life cycle: inflows and outflows of lead.



EM, emissions, I, inflow of goods into the stock, O, outflow or discarded goods, R, recycled stream, L, landfilled stream, IN, incinerated stream, S, stock of CRT, Imp, import, Exp, export.

### 4.3.1 The inflow of CRT into the societal stock

The inflow of CRTs into the product stock is calculated as the number of CRTs produced within the EU member states, plus the number of CRTs imported from outside the EU, minus the number of CRTs exported to non-EU countries. The inflow of CRTs is shown in Fig. 2 (CBS, 2000) and is expressed in terms of the lead it contains: in ktonnes of Pb. To model the inflow, we assume that the inflow of these products is affected by the availability of a viable substitute, by GDP, and by the size of the population.



**Fig. 2:** The inflow of CRT into the stock-in-use in the EU expressed in ktonnes of Pb.

#### *Gross Domestic Product (GDP)*

Gross Domestic Product (GDP) is a standard measure in monetary terms of economic production and, mirrored, income. Other variables, such as poverty and natural resources exploitation are intimately connected to it, either positively or negatively. On a general level, the correlation between GDP and production and consumption of products is valid by definition. For specific products such as CRT, televisions and computer monitors this relation can be more complex, as some products tend to be used less with higher incomes and others more.

#### *Population*

There are several reasons to consider population a determinant of the use of products. In the first place, there is the general law that it takes more to sustain more people. This refers mainly to the basic needs. Nowadays, televisions and computers are transferring from luxury goods to basic items and therefore a correlation between the population and the consumption of these goods can be expected.

#### *Substitution*

In the present CRT system, there seems to be no viable alternative for lead. There are some indications that lead could be replaced with other materials such as barium, strontium and zirconium, but no such glass is commercially available and it is not known if these materials can be supplied in sufficient quantities to meet the demand. It is likely that the use of cathode ray tubes will decline as a result of the rise of flat screen displays. When forecasting future inflows, this development can be included under various scenario assumptions.

### 4.3.2 The outflow of CRT from the societal stock

Since no emission of lead occurs during the use of CRT, the outflow of CRTs out of the stock is determined only by discarding: it equals the amount of the discarded CRT, including those in discarded TV's and PC monitors. The most important leakage to the environment probably will take place after the disposal stage in waste management and/including recycling. The average life time of CRTs is about 15 years (Tukker et al. 2001). At the moment, the stream of final CRT waste is split between landfill (80%) and incineration (20%) (Tukker et al. 2001). For electrical and electronic equipment, however, the future recycling rates are predicted to increase. Lead glass could be returned to glass manufacturers for recycling. At present, the glass industry is not doing this because there is no economic incentive to do so (Tukker et al. 2001). It is likely that the proposed EU Directive on Waste Electrical and Electronic Equipment (WEEE) will change this situation.

## 4.4 Empirical analysis and results

In this section, a preliminary empirical analysis of the CRTs inflow, outflow, stock and waste stream in the EU economy will be modelled and the model outcome will be discussed.

### 4.4.1 Modelling the inflow of the CRTs into the societal stock

To assess the relative importance of the explanatory variables for the CRT inflow, regression analysis is used. The independent variables used in the analysis are Gross Domestic Product (GDP), Population (Pop), and a Time variable (T) that will be used as a proxy for the combined influence of other variables on the inflow trend. The period of analysis was from 1988 to 1999. The fitting algorithm that determines the regression parameters ( $\beta_0, \beta_1, \beta_2, \beta_3$ ) in Eq. (7) uses the ordinary least square (OLS) criterion (Gijbels and Rousson, 2001).

$$Y(t) = \beta_0 + \beta_1 \cdot GDP(t) + \beta_2 \cdot Pop(t) + \beta_3 \cdot T(t) + \varepsilon(t) \quad (7)$$

where  $Y(t)$  is the inflow of goods at time  $t$ ,  $\beta_0$  is the overall mean response or regression intercept,  $\beta_1, \beta_2, \beta_3$  are the regression parameter or the main effect of the factors GDP, Pop, and T and  $\varepsilon(t)$  is the regression model error term

Table 1 shows the result of the regression analysis. Estimations 1 and 2 show a positive correlation between the GDP and population variables and the inflow, with a fairly high coefficient of determination ( $R^2_{adj}$ ). Estimation 3 shows a positive correlation between the inflow of CRTs and T. The correlation between the inflow of CRTs and all of the three variables separately is significant at the 95% probability level. The results indicate that the factors included in T (technological developments and substitution and maybe others) are important factors in the determination of the inflow shape, and therefore should be investigated further. The results show also that the coefficient  $\beta_3$  has a positive value which means the inflow will increase over time. This indicates that in the past, substitution has not had any influence on the inflow shape. In the future, this may be different. It is clear from the estimations 4, 5 and 6 that the combination between the variables is improving the overall correlation. When all the three variables are included in the regression model (estimation 7),  $R^2_{adj}$  has the highest value. The t test for the individual coefficients shows that in this model the GDP and population are not significant. The coefficient for population has an unexpected negative sign, though this coefficient is statistically insignificant. However, the F test indicates that all the independent variables taken together are significant and contribute to the shape of the inflow. Therefore, the following model will be used to calculate the inflow of the CRTs:

$$Inflow(t) = 9225 + 0.015GDP(t) - 25.42Pop(t) + 37.1T(t) \quad (8)$$

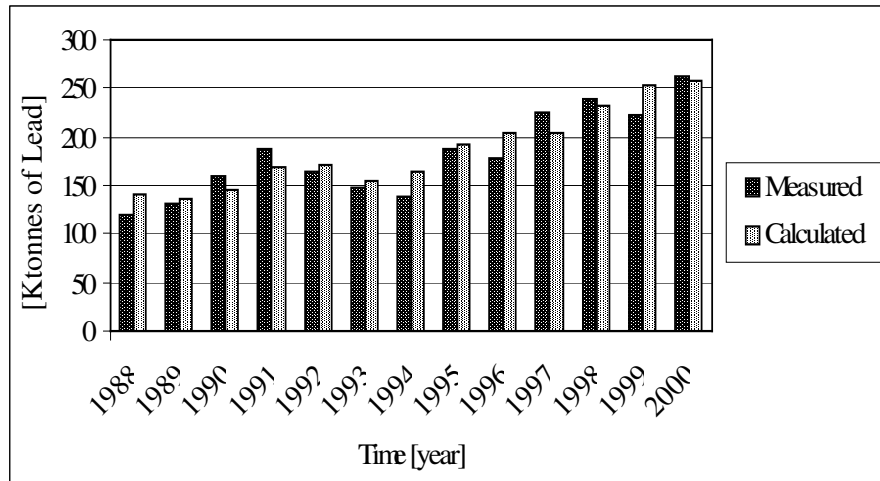
Figure 3 shows the difference between the measured inflow of CRTs and the calculated inflow from the regression model in Eq. (8).

#### 4.4.2 Modelling the outflow of CRTs from the societal stock

The outflow out of the CRT stock is the discarded CRTs, TVs and monitors. This flow is mainly determined by the life span of the CRTs in these applications. The life span is assumed to be distributed in time; a Weibull distribution is used assuming a minimum life span of 10 years and a maximum of 25 years, with a most likely life span of 15 years. The outflow is included in Fig. 4.

**Table 1:** Results of the analysis of the individual factors on the inflow of CRT

Estimation	Variables	$\beta_0$ (t-value)	$\beta_1$ (t-value)	$\beta_2$ (t-value)	$\beta_3$ (t-value)	$R^2_{adj}$	F statistics
1	GDP	47.4 (1.10)	0.01 (3.18)			0.43	10.15
2	Pop	2521 (-4.52)		7.3 (4.84)		0.65	23.49
3	T	111.76 (8.49)			9.97 (6.01)	0.74	36.23
4	GDP, Pop	-3351 (-2.64)	-0.008 (-0.73)	9.7 (2.67)		0.63	11.51
5	GDP, T	133.5 (3.51)	-0.004 (-0.61)		11.6 (3.63)	0.73	17.27
6	Pop, T	4811 (1.84)		-13 (-1.80)	26.5 (2.85)	0.78	23.46
7	GDP, Pop, T	9225 (2.20)	0.015 (1.32)	-25.42 (-2.17)	37.1 (3.08)	0.80	17.38



**Fig. 3:** Measured and calculated inflow of CRT, expressed in ktonnes of Pb

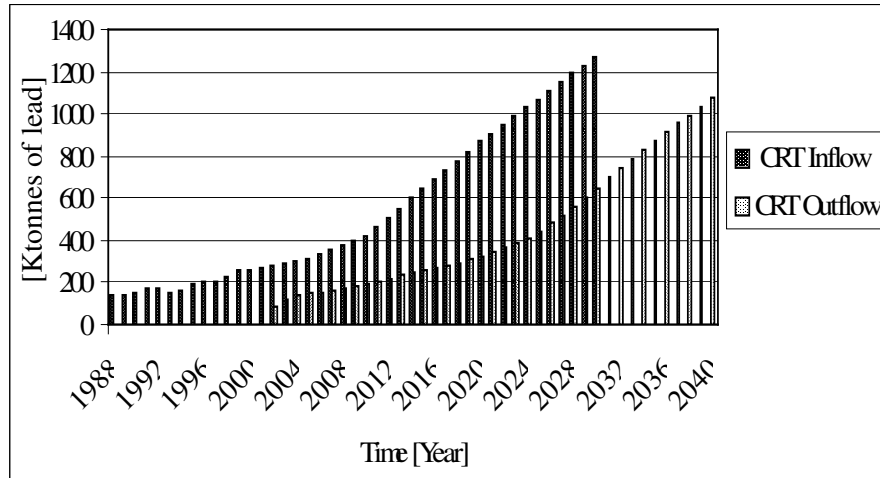
#### 4.4.3 Modelling the future inflow and outflow of CRTs

The future inflow of CRTs is calculated based on the regression model given by Eq. (8) and projected values of the variables GDP and population. Projections are taken from a study for the EU 6<sup>th</sup> Action Programme [9]. An average GDP growth for the EU by 2.4% per year is projected from 2001 to 2010; slowing to 1.8% per year between 2011 and 2020, and 1.7% per year between 2020 and 2030. The population of the EU is expected to increase slightly during the first decade of this millennium. After 2010, the rate of population growth falls and the population is expected to stabilize after 2020 [9]. The future outflow of CRTs is calculated from the past and future inflow of CRTs and the Weibull distribution of the

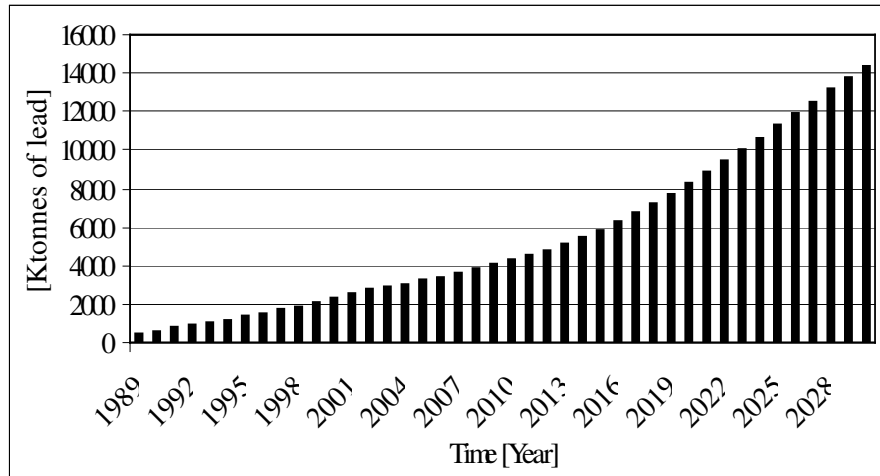
life span. Figure 4 shows the future inflow and outflow of the CRTs in the EU. The possible substitution of CRTs by flat screen displays is as yet ignored.

#### 4.4.4 Modelling the stock's size of CRTs

The only determinants of the change of the CRT stock over time as described by Eq. (6) are the stock's inflow and outflow, as calculated above. Additional information on the initial magnitude of the stock that is corresponding to the number of TVs and computers owned by people in the EU member states in 1988 is needed. These figures can be found in an UNDP overview (UNDP, 1992). The development in CRT stock size is shown in Fig. 5.



**Fig. 4:** Projected future inflow and outflow of CRT in the EU, expressed in ktonnes of Pb, based on “baseline scenario”, and Weibull distributed life span

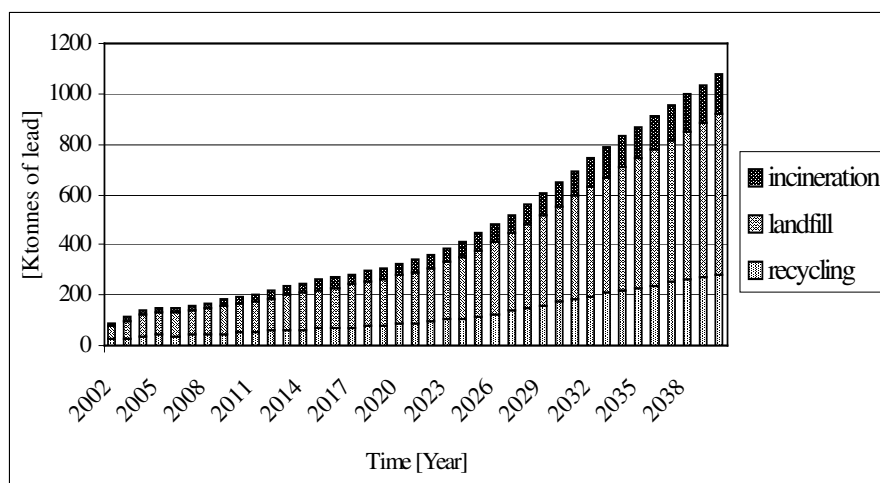


**Fig. 5:** Amount of lead in the CRT stocks in the EU

#### 4.4.5 Waste stream of CRTs

The draft WEEE states that of the equipment with cathode ray tubes that have been collected, 75% should be recycled or recovered. With a collection rate of 25% or 50% this implies overall recycling rates of 19 to 37.5%. An average value of 26.75% recycling rate has been used in modelling the future recycled stream. It

is also assumed that 80% of the remaining waste stream will be landfilled and 20% will be incinerated, which implies that 59% of the total discarded stream will be landfilled and 14.75% will be incinerated. The results of the calculations based on these assumptions are shown in Fig. 6.



**Fig. 6:** Future recycled, landfilled, and incinerated lead flows of CRT in the EU

## 4.5 Conclusions

1. The flows of a certain substance through the economy are basically determined by the economic demand for its applications. This implies that in order to model substance flows, the materials wherein the substance occurs should be a central modelling issue, in turn based on the analysis of the products containing these materials. In contrast, the outflow of the substance out of the economy in the shape of waste and emissions is basically determined by the physical-chemical properties of the substance. These properties determine the losses during use and the possibilities for recycling. A substance flow model therefore must include both economic and physical-chemical variables.
2. In this chapter, a method is presented to model the inflow of products, based on socio-economic variables such as GDP and population size. This method is applied to the case of lead applied in cathode ray tubes.
3. It appears that the model leads to good results: for a time series in the past, the measured inflow compares well to the modelled inflow. In principle, the same model can be used to estimate the future inflow. Not the measured GDP, population etc. but prognoses for these variables then must be used. The model forecasts however are only valid assuming that no unpredicted changes, such as the development of a completely new substitute, will occur. Changes like that will render the inflow model useless.
4. The time variable (T) is used as a proxy to capture the combined influence of other factors such as substitution and technical developments on the inflow. The results have shown that the time variable is an important factor in determining the inflow. The variables implicitly included in T should be investigated further. These variables include technical developments but especially substitution and the driving forces behind that, such as the price of the product or the raw materials and energy embedded in it.
5. In addition, a method is presented to model the product outflow based on two mechanisms: leaching and delay. Leaching refers to emissions of the substance during the use of a product, i.e. by corrosion or volatilisation, and is modelled as a fraction of the total stock of products-in-use. Delay refers to the discarding after use of products, and is determined by the life span of the products. Different distributions can be chosen. In the case of lead in cathode ray tubes, a Weibull distribution was used. The results of the outflow model have not been compared yet with real data.

## 4.6 Outlook

The model presented in this chapter is a dynamic stock model based on product stock characteristics. The model is meant to be an integral part of a general dynamic substance flow model that can be used to estimate the total environmental consequences of the use of substances in the economic system. At this stage, the model is capable of investigating the main factors determining the dynamic behaviour of a substance, namely the stocks of products containing the substance and its inflows and outflows. The next step is to integrate the models for the different products into one framework at the substance level. The idea is that the result will be more than the sum of its parts. On the one hand, the flow of the substance is also determined by certain characteristics, which can be both functional and economical. On the other hand, recycling can be modelled most adequately at the substance level. In the case of lead, many products contribute to the availability of secondary lead, while the demand for primary lead is influenced by the recycling flow as a whole. This will be the subject of further research. Finally an integration of the substance stock model with a substance flow model will be attempted. The final dynamic substance flow-stock model should include in addition to the use phase, the extraction, manufacturing and waste treatment activities. The stock model should be the central module. For a complete analysis of the environmental consequences of substance flows and stocks in the economic system the energy use in different stages of the system should also be accounted for.

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## **Chapter 5    The Environmental and Economic Consequences of the Developments of Lead Stocks in the Dutch Economic System \***

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### **Abstract**

This chapter investigates the developments of lead stocks in the Dutch economy and the consequences of such developments for the environment and the economy. The analysis is based on a dynamic substance stock model that combines physical and socio-economic elements. The model estimates lead demand in different applications as a result of the developments in the socio-economic variables. In addition, it estimates the current and future size of lead stocks, the future outflow of discarded lead applications and related emissions, and the availability of lead for future recycling based on the life span, corrosion rate and recycling rate of the lead applications. The results show that the lead inflow is determined by the demand for its individual applications, which in turn are mainly determined either by per capita GDP or by population growth. In future, the societal stock is expected to change from a lead sink to a lead source. The future availability of lead for recycling will exceed its demand. This implies that lead demand in the Netherlands can be met completely by secondary sources. If a similar trend can be found in other countries, a situation of oversupply may arise with adverse consequences for the recycling business and ultimately for the emissions of lead to the environment.

### **Keywords**

Substance Flow Analysis; Dynamic Stock Modelling; socio-economic; Lead; Recycling; Resources

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\* Reprinted from “Elshkaki, A., Van der Voet, E., Van Holderbeke, M., and Timmermans, V. (2004). Resources, Conservation and Recycling; 42: 133-154”.

## 5.1 Introduction

Over the last century, the increase of the global population and the growth of the economic activities have been accompanied with an increase of materials demand, and consequently with an increase of extracting, processing, using and waste treatment activities. This has raised the concern about the depletion of resources and the emissions during resources life cycle especially those of heavy metals.

Environmental policies aiming at the reduction of the emission of heavy metals include end-of-pipe processes, but also more integrated measures like the stimulation of recycling and the phasing out of hazardous intended (e.g. lead in gasoline) or not-intended (e.g. cadmium in phosphate fertilizer) applications. Although these policy measures seem to be effective on the short term, their effectiveness on the long term is questionable. A well-known example concerns cadmium recycling. On the short term, recycling may reduce cadmium emissions, however, on the long term these emissions will increase due to the fact that the inflow of cadmium into the economy is supply driven (Huppel et al. 1992). This implies that a reduced demand does not result in a reduced supply. A comparable example concerns mercury. The demand for mercury has decreased so much as a result of a strict policy, that its supply can be covered completely from by-product sources, such as from the purification of natural gas. In this case, policies aimed at phasing out or recycling mercury applications therefore will lead to an increase of its stock in society (Maxson et al. 1991).

This chapter investigates the dynamic behavior of lead stocks in the Dutch economy. Lead has been chosen because it is one of the most extensively used heavy metals in the economic processes on the one hand, and because of its toxic characteristics and its accumulation in the economy on the other hand (Scoullios et al. 2001). In the Netherlands, policy aims at a reduction of lead emissions by phasing out certain lead applications and increasing recycling. On the short term, the phasing-out policy has resulted in a reduction of lead emissions (Tukker et al. 2001), while recycling has led to a reduced landfill of lead containing waste. On the long term, however, both types of measures may have unexpected and undesirable side effects, comparable with cadmium and mercury.

The present chapter investigates the consequences of the past and future developments of lead stocks on the long-term lead management. The cases of cadmium and mercury as mentioned above have been analyzed using Substance Flow Analysis (Van der Voet 1996). These analyses are based on static modelling. It is argued, however, that for long-term management, information is required on the dynamic behavior of substances in the economy (Guinée et al. 1999). Recently, it is acknowledged that including the dynamics in the system is connected to the inclusion of stocks in society (Bergbäck and Lohm 1997). The dynamics of such stocks are very important for the generation of future waste and emissions. Considering stocks so far has resulted in a few specific substance stock inventories or models (Boelens and Olsthoorn 1998; Kleijn et al. 2000). The analysis in this chapter is carried out using a general dynamic substance stock model that combines physical and socio-economic elements.

The chapter is structured as follows. Section 2 will outline the dynamic stock model. In Section 3, a description is presented of the lead applications and the past and future inflows, outflows, and wastes streams of lead are quantified. Section 4 contains the results of the model calculations and Section 5 is dedicated to discussion and conclusions.

## 5.2 Dynamic stock model

Stocks in society refer to the materials, products and infrastructure in use. Large and increasing amounts of materials are stored in such stocks. Stocks of lead can be found, for example, in buildings and in cars. Stocks can be regarded as buffers in the economic system, causing a delay between the inflow of new products and the outflow of discarded products. Phasing out policies aimed at stockbuilding applications thus will become effective only after a certain delay, which could be considerable depending on the exact application.

In general, a substance or material stock is composed out of all the products that contain the substance or material and have a life span longer than 1 year. This could be a large number of products with widely different behavior. This implies that a substance stock model should at least contain two layers: the substance level and the product level. Products are associated with a demand and have a life span, which may or may not be influenced by the substances it contains. A substance in a product may be substituted without changing the demand for the product. The substance in a waste product may be extracted and

recycled, and subsequently applied in different products. As a result, the substance leaves the specific product stock but not society, and the life span of the substance may differ considerably from the life span of each of its applications.

Stocks are continuously renewed. On the one hand, old products are discarded from the stock. On the other hand, new products are bought and become part of the stock. The stock dynamics are determined by this process of renewal. Below, the modelling of the inflow and outflow of the stock is described.

### 5.2.1 Modelling the stock's inflow

The inflow of a certain substance into a stock-in-use is primarily determined by the demand for the products containing the substance. The demand is influenced by socio-economic or economic factors such as Gross Domestic Product (GDP), per capita GDP, population size and growth, inter- and intrasectoral share in GDP, price, consumer taste and preference, substitution and technical developments. In the model, a general function is used to describe the inflow, which is fitted for each product separately based on past trend data (Elshkaki et al., 2002):

$$F^{in}(t) = \beta_0 + \sum_{i=1}^n \beta_i X_i(t) + \varepsilon(t) \quad (1)$$

where  $F^{in}(t)$  is the inflow into the product stock at time  $t$ ,  $n$  is the number of explanatory variables,  $X_i(t)$  is the socio-economic variable at time  $t$ ,  $\beta_i$  is the model parameter and  $\varepsilon(t)$  is the model error at time  $t$ .

Sometimes the demand in a certain year does not correspond to the change in the socio-economic variables in the same year, but to changes in these variables some years earlier. Apparently, there is sometimes a time lag between the driving forces and the response. In a mathematical form, this time lag could be accounted for as given by Eq. 2:

$$F^{in}(t) = \beta_0 + \sum_{i=1}^n \beta_i X_i(t-j) + \varepsilon(t) \quad (2)$$

where  $X_i(t-j)$  is the socio-economic variable at time  $(t-j)$ ,  $j$  is the time lag.

### 5.2.2 Modelling the stock's future inflow

The derived inflow model described by Eq. 1 or 2 can be used further to estimate the future inflow of goods. Projected values of the influential variables are then required. Such projections are available for GDP and population in different scenario studies (RIVM 2000). The assumption then is that there is no discontinuity changing the dependency of the demand on the influential variables.

### 5.2.3 Modelling the stock's outflow

The outflow out of the stock takes place through two processes: leaching and delay (Van der Voet et al. 2002). Leaching occurs during use due to corrosion or slow volatilization of substances from various stocks of applications. These emissions may end up in the soil, surface water, groundwater or sewage system. The yearly emissions of a substance in a certain application can be modelled as a fraction of the total size of the stock by linear or exponential emission coefficients. In the model, a linear emission coefficient is used as given by Eq. 3.

$$F^{out}_E(t) = C \cdot S(t) \quad (3)$$

where  $F^{out}_E(t)$  is the outflow due to emissions at time  $t$ ,  $C$  is the emission factor and  $S(t)$  is the stock at time  $t$ .

Delay is related to the discarding of products after use. The discarded outflow of a certain product depends mainly on the product inflow and its life span. The empirical data on the life span is often not available. In

that case, the alternative is to assume either an average life span or a certain life span distribution. The discarded outflow could be modelled as a delayed inflow, corrected for the emissions that have taken place during use, as given by Eq. 4:

$$F^{out}_D(t) = F^{in}(t-L) - \sum_{i=1}^L C \cdot F^{in}(t-L) \cdot (1-C)^{i-1} \quad (4)$$

where  $F^{out}_D(t)$  is the outflow due to the delay mechanism at time  $t$ ,  $C$  is the emission factor and  $L$  being the average life span of the product.

The total outflow at time  $t$ ,  $F^{out}$  then is given by Eq. 5

$$F^{out}(t) = F^{out}_D(t) + F^{out}_E(t) \quad (5)$$

### 5.2.4 Modelling the stocks

The change of the magnitude of the stock over time is the difference between the inflow and the outflow as given by Eq. 6.

$$\frac{dS}{dt} = F^{in}(t) - F^{out}(t) \quad (6)$$

By knowing the initial value of the stock and the inflow of goods, it is possible to calculate the stock as given by Eq. 7.

$$S(t+1) = S(t) + F^{in}(t) - F^{out}(t) \quad (7)$$

### 5.2.5 Modelling the waste streams

The discarded outflow ( $F^{out}_D$ ) will be partly recycled and partly will end up in final waste treatment, either on landfill sites or in incineration plants. Recycled, incinerated, and landfilled streams can be modelled as a fraction of the discarded outflow as given by Eqs. 8, 9 and 10.

$$R(t) = a_1 \cdot F^{out}_D(t) \quad (8)$$

$$L(t) = a_2 \cdot F^{out}_D(t) \quad (9)$$

$$I(t) = a_3 \cdot F^{out}_D(t) \quad (10)$$

where  $R(t)$ ,  $L(t)$ , and  $I(t)$  are recycled, landfilled and incinerated streams at time  $t$ . The parameters  $a_1$ ,  $a_2$ ,  $a_3$  are recycling, landfilling, and incineration fractionation ratios. These fractionation ratios in reality depend on many technical, economical and policy factors.

## 5.3 Description and modelling of lead applications in the Dutch economy

### 5.3.1 Systems definition

Refined lead originates from primary and secondary sources. The most common primary source of lead is galena (lead sulphide, PbS). Lead is often found associated with other heavy metals such as zinc, copper, silver and bismuth. Lead ore is the main source of silver (Scoullou et al. 2001) and bismuth (Graedel 2002). The main source of secondary lead is the recycling of its applications, mainly batteries and lead sheet.

Lead is one of the most extensively used heavy metals in society due to its unique properties such as conductivity, corrosion resistance, density, flexibility, durability and attractive appearance. The largest

application of lead is its use in batteries. Lead in batteries is applied in a variety of products: starting, lighting and ignition (SLI) batteries, traction or stationary batteries and industrial batteries. Traction batteries refer to those batteries that are used to power electric vehicles. The second largest application is lead sheet in building. The third largest application is as a pigment in cathode ray tubes as applied in televisions and computer monitors. Cable sheathing, also a lead containing product, is used for indoor electricity cables in buildings and outdoor electricity, telephones and gas pipes. In the past this used to be a large application. Now it is phased out completely, at least in the Netherlands (Tukker et al. 2001), although still present in old stocks. Furthermore, lead is applied in a number of small products that are used in vehicles such as electronics, wheel weights, glazes, light bulbs, and bronze bushings and bearings. We will refer to this as “Non–battery vehicle applications”.

In addition to its intentional use, lead is present in several products as a contaminant. Lead occurs naturally in trace concentrations in fossil fuels and in phosphate rock. Via phosphate fertilizer it enters the agricultural chain and accumulates there. As a result of processing lead containing waste, it also occurs in residues of waste management such as sewage sludge, compost and products of incineration, i.e. fly ash and bottom ash. These residues sometimes are put to use again. The lead thus enters a secondary, non-intentional life cycle. Fly ash and bottom ash, for example, are used as materials in road construction.

In this chapter, the above-mentioned intentional applications, which account for more than 95% of the total lead inflow in the Dutch economy, are included. They are all applications relevant for a stock model, since their life span exceeds 1 year. The non-intentional applications are not included in the model, because they are generally not associated with stock building. Fig. 1 shows the system of lead flows and stocks in the Dutch society. The stock model as described in Section 2 refers to the stocks-in-use, with their inflows and outflows, as indicated in Fig. 1.

The variables and parameters of the Dutch lead stock model will be described in the following sections.

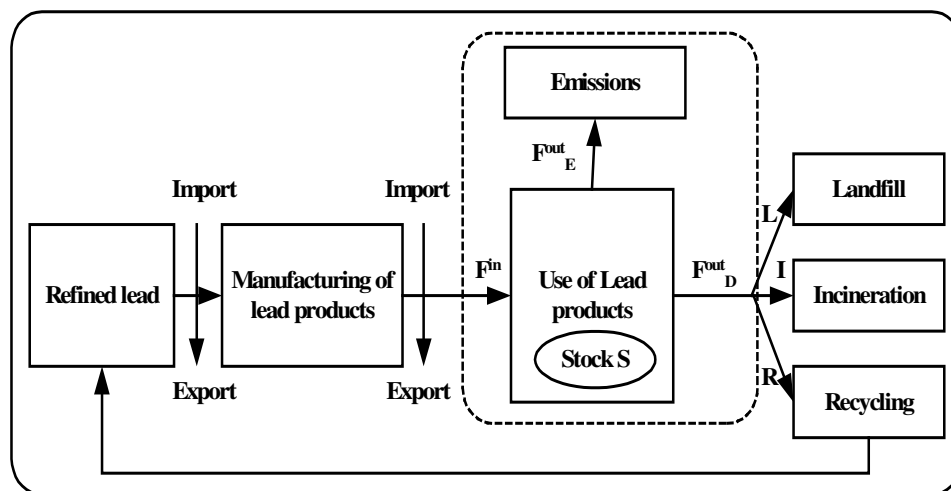


Fig. 1: Overall structure of the model.

The consumption phase of the Dutch economy is marked with a dashed line

### 5.3.2 Quantification of the past inflow of lead applications

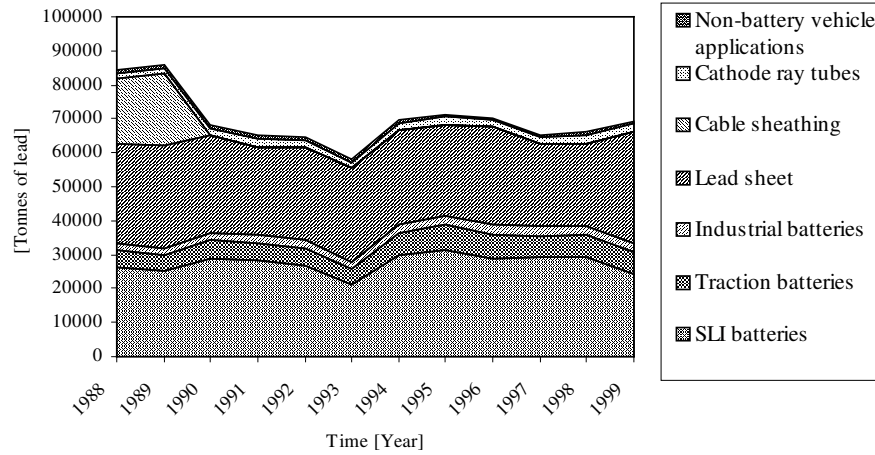
Fig. 2 shows the past inflow of lead into the stock of products-in-use in the Netherlands from 1988 through 1999.

#### *Battery system*

The inflow of lead in batteries into the consumption phase is quantified as the number of batteries multiplied by the fraction of the weight that is taken by lead. The lead content of typical SLI, traction or industrial batteries is about 58% of their weights. The inflow of SLI, traction and industrial batteries into

the stock-in-use from 1988 through 1999 (Fig. 2) (CBS, 2000; ILZSG, 2000) is the number of produced batteries plus imported batteries minus exported batteries. SLI and traction batteries enter the economy either as separate products or combined with other products, mainly vehicles. The number of SLI and traction batteries corresponding to those products is accounted for as given by Eq. 11.

$$F^{in}(t) = production(t) + [import(t) - export(t)]_{batteries} + [import(t) - export(t)]_{vehicles} \quad (11)$$



**Fig. 2:** Past inflow of lead products into the stock of products-in-use in the Netherlands, 1988-1999

### **Lead sheet in building**

The inflow of lead sheet is quantified in two steps. First, from 1988 through 1999 (Fig. 2) (CBS, 2000; ILZSG, 2000), the inflow is quantified as the produced amount plus the imported minus exported amounts as give by Eq. 12. Second, from 1950 through 1987, the inflow is quantified as the inflow of lead sheet in houses and utility buildings. Lead sheet inflow in houses is quantified based on the newly built houses (Eurostat, 2000) multiplied by an average amount of lead per house. The average amount of lead in each house is estimated as the inflow from 1988 through 1999 divided by 2 (assuming 50% of the inflow is used in houses) divided by the number of newly built houses. The average amount of lead in houses thus is calculated to be 146.95 kg/house.

$$F^{in}(t) = production(t) + [import(t) - export(t)] \quad (12)$$

### **Cable sheathing**

The inflow of indoor cable sheathing from 1950 through 1970, is quantified based on newly built houses (Eurostat, 2000) and an assumption that the amount of lead in cable sheathing equals 1.5 kg/house (Palm, 2002). In the case of outdoor cable sheathing, no information is available that can be used directly to quantify the inflow. However, information is available that can be used to quantify outdoor cable sheathing outflow and stock. The inflow thus can be quantified based on the outflow and the stock. The inflow of outdoor cable sheathing from 1960 through 1990 is quantified as net inflow plus outflow as given by Eq. 13. The net inflow is the difference between stocks in two consecutive years as given by Eq. 14. Cable sheathing outflow and stock are estimated in sections 3.4 and 3.5. Lead is phased out from indoor cable sheathing in 1970 and from outdoor cable sheathing in 1990.

$$F^{in}(t) = F^{net}(t) + F^{out}(t) \quad (13)$$

where  $F^{in}(t)$  is the inflow of outdoor cable sheathing at time  $t$ ,  $F^{net}(t)$  is the net inflow at time  $t$ , and  $F^{out}(t)$  is the outflow of outdoor cable sheathing at time  $t$ .

$$F^{net}(t) = S(t+1) - S(t) \quad (14)$$

where  $S(t)$  is the stock of outdoor cable sheathings at  $t$ , and  $S(t+1)$  is the stock at time  $t+1$ . Substitution of Eq. 14 in Eq. 13 gives

$$F^{in}(t) = S(t+1) - S(t) + F^{out}(t) \quad (15)$$

### ***Cathode Ray Tubes (CRTs)***

Lead inflow in televisions CRTs from 1976 through 1999, in household computers CRTs from 1988 through 1999, and in office computers CRTs from 1989 through 1999 (Fig. 2) is quantified, in the same manner as outdoor cable sheathing, as given by Eq. 15. A CRT contains about 2 kg lead. CRTs outflow and stock are estimated in sections 3.4 and 3.5.

### ***Non-battery vehicle applications***

The inflow of lead in non-battery vehicle applications (Fig. 2) is quantified as the amount of lead corresponding to the amount or the number of these application in one vehicle (Lohse et al. 2001) multiplied by the number of newly registered vehicles (CBS, 1987-2000).

The amount of lead used per weight for wheel balancing lies between 20 and 25 g as an average. As each vehicle is equipped with 10 weights, this sums up to 200-250 g lead per vehicle. In this study an average of 225 g has been used. Lamps in vehicles contain between 0.2 and 0.75 g lead in the glass bulb, and solder contributes up to 0.2 g lead per lamp. As an average value of 0.4 to 0.5 g lead per bulb is stated. An average vehicle is equipped with 30 to 40 lamps, these sums up to 12-20 g lead per vehicle. Electronics contain about 52.7 g of lead per vehicle. Glazes contain about 1.2 g of lead per vehicle. Bronze bearings and bushings contain about 10 g of lead per vehicle (Lohse et al. 2001). In total, a vehicle thus contains ca. 300 g of lead in small applications.

## **5.3.3 Estimation of future inflow of lead applications**

The future inflow of lead into the stock of products-in-use for batteries, lead sheet and non-battery vehicle applications is estimated in two steps. Firstly, we used the regression model as given by Eq. 2 to describe the relationship between the past inflow of lead in each product from 1988 through 1999 and the socio-economic variables (GDP, per head GDP, sectoral share in GDP, lead price, and population size and growth). The regression analysis enables us to test the most significant variables among the socio-economic variables and to eliminate those that do not correlate with the past inflow of the products. The adequacy of the model and the significance of the individual variables are evaluated based on statistical terms such as the adjusted coefficient of determination  $R^2_{adj}$ , the t-test and the F-statistics. The inflow model equation for each of the lead products as a result of the regression analysis is given in table 1. The results of the regression analysis show that the population size, population growth and per head GDP are the most significant variables. Other variables such as GDP, sectoral share in GDP and lead price are either do not correlate with the inflow (i.e. the adjusted coefficient of determination is low) or insignificant when combined with other variables. Secondly, we used scenario projections of the future development in the most significant variables in the regression model to estimate the future inflow. The projections for the socio-economic variables can be found in (RIVM, 2000). For CRTs, the regression model given by Eq. 2 is used to estimate a relation between the stock of CRTs and the different socio-economic variables.

As has been mentioned in section 2.1, other factors such as consumer's taste and preference, technical development and substitution may affect the inflow, however, these variables are not included in the analysis.

### ***Battery system***

On a product level, the increase or decrease of Gross Domestic product (GDP) can hardly explain the SLI batteries past inflow trend. The production of lead batteries for new vehicles is expected to fluctuate with the business cycle, but this will not be the case for replacement batteries, which constitute the largest part of the lead batteries market (Tilton, 1999). The results show that this trend could be explained by population growth with a time delay. This is possibly due to an effect of population development on

vehicles sales market and their use. The slightly increasing inflow of industrial batteries could be explained by the developments in the population size but could be explained much better by per capita income development. Per capita income fluctuates in line with the inflow most of the time. Traction batteries are used in different applications with different behavior. Some of them could be effected by the economic growth and others by population developments.

**Table 1:** The inflow model equation for each of the lead applications

Application	The inflow equation	R <sup>2</sup>	F-Statistics
Batteries			
SLI batteries <sup>a</sup>	$\text{Inflow}(t) = 18756.0 + (0.0957 * \text{PopGrowth}(t-4))$	0.34	5.3
Traction batteries	$\text{Inflow}(t) = 236.5 + (0.0261 * \text{GDP/capita}(t))$	0.76	32.0
Industrial batteries	$\text{Inflow}(t) = 783.0 + (0.0076 * \text{GDP/capita}(t))$	0.69	22.3
Lead sheet	$\text{Inflow}(t) = 21583.0 + (0.0651 * \text{PopGrowth}(t-14))$	0.6	13.5
Cathode ray tubes (CRTs)			
CRT- Televisions	$\text{Stock}(t) = -1.19\text{E}7 + (1.1760 * \text{Pop}(t))$	0.97	447.0
CRT- Household computer	$\text{Stock}(t) = -4.27\text{E}7 + (2.9420 * \text{Pop}(t))$	0.96	312.0
CRT- Offices computers	$\text{Stock}(t) = -2.62\text{E}7 + (1.8270 * \text{Pop}(t))$	0.99	1356.0
Non-battery vehicle applications			
Electronics	$\text{Inflow}(t) = 109.0 + (0.000352 * \text{PopGrowth}(t-12))$	0.55	15.1
Bronze, bearing and bushings	$\text{Inflow}(t) = 20.68 + (0.000067 * \text{PopGrowth}(t-12))$	0.55	15.1
Glazes	$\text{Inflow}(t) = 02.48 + (0.000008 * \text{PopGrowth}(t-12))$	0.55	15.1
Light bulbs	$\text{Inflow}(t) = 24.82 + (0.000080 * \text{PopGrowth}(t-12))$	0.55	15.1
Weight wheels	$\text{Inflow}(t) = 465.0 + (0.001505 * \text{PopGrowth}(t-12))$	0.55	15.1

<sup>a</sup> Starting, lighting and ignition

### ***Lead sheet in building***

The inflow of lead sheet in buildings is directly linked to housing demand, which is mainly driven by the growing population.

### ***Cathode Ray Tubes (CRTs)***

The demand for CRTs is determined by the demand for televisions, household computers and office computers. The demand for televisions was expected to be driven by the population growth whereas the demand for household computers could be driven by both population growth and economic growth. However, it was difficult to find an equation that can fit the past inflow of televisions and computers. Therefore, we analyzed the relation between the stock size and the socio-economic variables. The results show that the televisions and computers stock size significantly correlate with all of the considered variables. However, the best correlation is the one with the population size. Moreover, the results show that R<sup>2</sup>adj and F-statistics associated with the three correlation are different. This variation is due to the difference in the three stocks. Although the stock of televisions and the stock of household computers are estimated based on the same number of household, the percentage of households owning a television and those owning a computer are changing overtime in a different manner.

### ***Non-battery vehicle applications***

The demand for Non-battery vehicle applications is directly linked to the demand for vehicles, which is mainly determined by population growth and economic growth. The results of regression analysis show the same statistical terms for all non-battery vehicle applications. This is due to the procedure followed in the quantification of their past inflow. The inflow of non-battery vehicle applications is estimated based on the



number of newly registered vehicles, which is applied for all these applications, multiplied by the number or the amount of these applications in one vehicle, which is constant overtime.

### 5.3.4 Estimation of the past and future outflow of lead applications

The outflow of lead applications is the sum of the outflow of discarded products and the outflow due to emissions during use. The discarded stream is estimated from the past and future inflow and products life span as given by Eq. 4. The emitted outflow is estimated as a fraction of the stock as given by Eq. 3.

For some applications such as lead sheet, cable sheathing and cathode ray tubes, the outflow will be affected by the initial stock (the stock generated before the available statistical figures of the inflow). The outflow due to the initial stock will be calculated separately, since Eqs. 3 and 4 are not applicable: the age distribution of the initial stock is unknown. It is assumed that the initial stock will be completely discarded and emitted in a number of years, namely the most likely life span for each of these applications (Table 2). Ultimately, the outflow in a certain period is the sum of the outflow due to the initial stock and the outflow due to the known past inflow. The inflows of different applications are those quantified in sections 3.2 and the emission factors and life span for lead applications are given in table 2. The life span is assumed to fit a Weibull distribution. Weibull distribution has been used because it has been shown experimentally that it provides a good fit for many types of life span (Melo, 1999).

**Table 2:** The emission factors, life spans and waste stream distributions of the different lead applications

Application	Minimum life span (year)	Maximum life span (year)	Most likely life span (year) <sup>b</sup>	Emission during use (%)	Recycling (%) <sup>b</sup>	Incineration (%) <sup>b</sup>	Landfilling (%) <sup>b</sup>
<b>Batteries</b>							
SLI <sup>a</sup>	4	7	5	0	95	3.5	1.5
Traction	3	8	5	0	95	3.5	1.5
Industrial	3	12	10	0	100	0	0
<b>Lead sheet</b>	45	75	50	0.008 <sup>b</sup>	90	2	8
<b>Cables</b>							
Indoor	20	45	30	0	75	-	-
Outdoor	20	45	30	0.025 <sup>c</sup>	75	-	-
<b>CRT</b>	10	25	15	0	50	15	35
<b>Non-battery applications</b>	2	20	12	0	0	25	75

<sup>a</sup> Starting, lighting and ignition

Sources: <sup>b</sup> Tukker et al. 2001, <sup>c</sup> Palm 2002

#### **Battery system**

The outflow of batteries is only the waste stream. It is assumed that there is no emission during the use phase. The waste stream is estimated as given by Eq. 4.

#### **Lead sheets in building**

The outflow of lead sheet from stock is the waste flow due to demolishing of buildings or renewing and replacement of sheets. Emission during use takes place as a result of corrosion. The outflow is estimated in two steps because the outflow from the initial stock needs to be calculated separately. First, from 1950 through 1999, the outflow of discarded lead sheet from the initial stock in 1950 is estimated as given by Eq. 16 below, with  $\alpha = 0.02$ . Second, from 1996 onward, this outflow is estimated as given by Eq. 4. The second step started at 1996 due to the minimum life span of lead sheet in buildings (45 years) and the first available inflow in 1950. The emissions during use from 1950 onward are estimated as given by Eq. 3.

$$F_{D}^{out}(t) = \alpha \cdot [S(1950) - (L_m \cdot C \cdot S(1950))] \quad (16)$$

$$\alpha = 1/L_m \quad (17)$$

where  $F_{D(t)}^{out}$  is the discarded outflow at time  $t$ ,  $L_m$  is the most likely life span and  $C$  is the emission factor

### ***Cable sheathing***

The outflow of cable sheathing is broken down into the outflow of indoor and outdoor cable sheathing. The outflow of both is estimated in two steps as the discarded sheathings due to demolishing buildings or replacing cables, and the emissions during use for the outdoor cables. The outflow of indoor cables is only the waste stream. It is assumed that there is no emission during the use phase. The outflow of waste indoor cables from 1950 through 1980 is estimated as a fraction of the initial stock in 1950, as given by Eq. 16 with  $\alpha = 0.033$ . From 1970 onward, the waste stream is estimated as given by Eq. 4. The outflow of waste outdoor cables from 1960 through 1990 is estimated as a fraction of the initial stock of 1960, as given by Eq. 16 with  $\alpha = 0.033$ . From 1980 onward, the waste stream is estimated as given by Eq. 4. The emissions from 1960 onward are estimated as given by Eq. 3.

### ***Cathode Ray Tubes (CRTs)***

The outflow of CRTs is only the discarded stream with televisions and computers, because no emissions occur during their use phase. The amount of discarded lead in CRTs in televisions as well as in household and office computers are each estimated separately in two steps using the same procedure for the first ten years. First, discarded CRTs from the initial stock in 1975, 1987 and 1988 for televisions, household computers and office computers respectively are estimated as given by Eq. 16. For each of these applications,  $\alpha = 0.06$  in Eq. 16. Next, discarded CRTs are estimated as given by Eq. 4.

### ***Non-battery vehicle applications***

The outflow of non-battery vehicle applications is the discarded amount with discarded vehicles. The life span of these applications is assumed to be the same as the life span of the vehicle. The stream of discarded non-battery vehicle applications is estimated as given by Eq. 4. It is assumed that no emissions occur during their life time.

## **5.3.5 Estimation of the stocks of lead applications**

### ***Battery system***

The initial stock of lead in SLI batteries in 1998 (Table 3) is estimated as a fraction of the weight that is taken by lead (58%) multiplied by the total number of vehicles in 1998. The development of the stock of lead in batteries from 1998 onwards is estimated as given by Eq. 7.

### ***Lead sheets in building***

The initial stock of lead sheet in buildings in 1950 (Table 3) is estimated as an average amount of lead of 146.95 kg per house multiplied by total number of houses in 1950, and consequently multiplied by 2 to correct for utility buildings. The development of the stock of lead sheet from 1950 onwards is estimated as given by Eq. 7.

### ***Cable sheathing***

The initial stock of lead in indoor cable sheathing in 1950 (Table 3) is estimated as an average amount of lead of 1.5 kg per building multiplied by the number of houses in 1950, again multiplied by 2 to correct for utility buildings. The stock of lead in indoor cable sheathing after 1950 is estimated as given by Eq. 7.

The lead stock in outdoor cable sheathing from 1960 through 1990 is estimated as an average amount of lead of 16.7 kg per capita in electricity cables and 12.8 kg per capita in telephones and 0.173 kg per capita in gas pipes, multiplied by the population size (Palm, 2002). The same procedure is used to estimate the initial stock in year 1960 (Table 3). After 1990, the stock is estimated as given by Eq. 7.

### ***Cathode Ray Tubes (CRTs)***

The lead stock in CRTs in televisions in the period from 1975 through 1999 is estimated as an average amount of lead of 2 kg per television, multiplied by the number of televisions in stock. In turn, the stock of televisions is estimated as the number of household multiplied by the percentage of households owning a

television (CBS, 1975-2000). The same procedure is followed for the estimate of lead stock in CRTs in household computers in the period from 1987 through 1999. For office computers, the number is known and could be applied directly (CBS, 1987-2000). The initial stock of lead in CRTs is the one estimated for the year 1999 (Table 3). After 1999, the stock is estimated as given by Eq. 7.

### ***Non-battery vehicle applications***

The initial stock of lead in non-battery vehicle applications in 1998 (Table 3) is estimated as an average amount of lead per vehicle multiplied by the number of vehicles in 1998. The stock of lead in non-battery vehicle applications from 1998 onwards is estimated as given by Eq. 7.

**Table 3:** The initial stock of lead in its different applications

Application	Year	Initial stock (tones of lead)
Starting, lighting and ignition (SLI) batteries	1998	45600
Lead sheet	1950	640000
Indoor cable sheathing	1950	6530
Outdoor cable sheathing	1960	341000
Non-battery vehicle applications	1998	1800
Cathode ray tubes	1999	26700

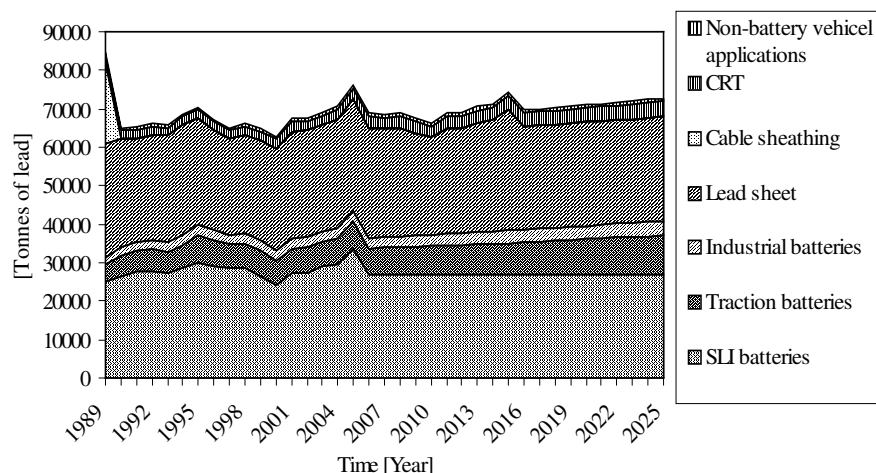
### **5.3.6 Estimation of the waste streams of lead applications**

The lead discarded from the stock of products-in-use will be partly recycled and will partly end up in the final waste treatment, either in landfill sites or in incineration plants. These streams are modelled as given by Eqs. 8, 9 and 10. The discarded outflows are those estimated in section 3.4. The recycling fraction ( $a_1$  in Eq. 8), landfill fraction ( $a_2$  in Eq. 9) and incineration fraction ( $a_3$  in Eq. 10) are given in table 2 (Tukker et al. 2001). We assumed that these fractionation ratios will remain the same in the future.

## **5.4 Results**

### **5.4.1 Past and future inflow of lead applications**

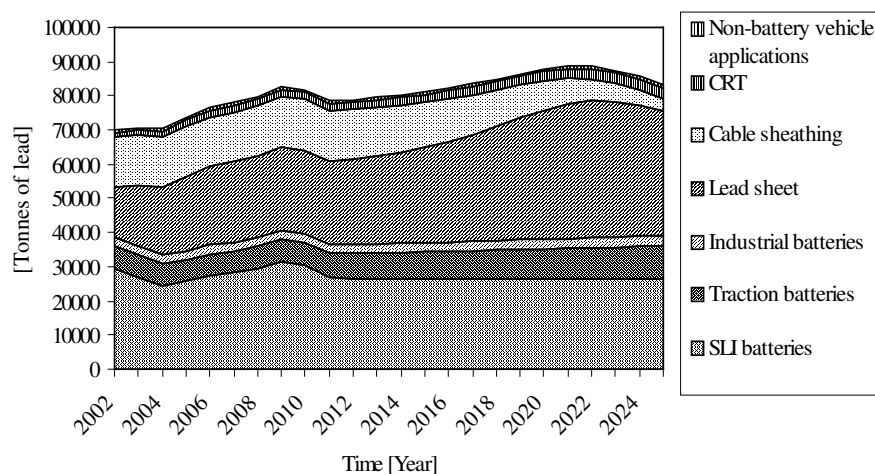
The results of application of the product stock models described in section 3 show that the inflow of lead in the Dutch economy can be better explained on a product basis than as a total lead inflow due to the number of lead applications, and the different behavior of each application. Fig. 3 shows the total past and future inflow of lead into the stock of products-in-use from 1989 to 2025, broken down to the different applications. The future inflow of SLI batteries is expected to increase from 2000 through 2006 and to stabilize after 2006. The future inflow of industrial batteries and traction batteries are expected to increase over time. The demand for lead sheet is expected to stabilize in the future as a consequence of the stabilization in the demand for houses. In the future, the demand for computers is expected to increase significantly whereas the demand for televisions will be increasing only slightly. The inflow of non-battery vehicle applications is expected to increase from 2000 through 2013 and to stabilize after 2013. In all, the applications for which the inflow can be related to the population growth are expected to stabilize in the future, while the GDP dependent applications will increase further. This is easily explained by the projected development of population and GDP in the RIVM scenario (RIVM, 2000).



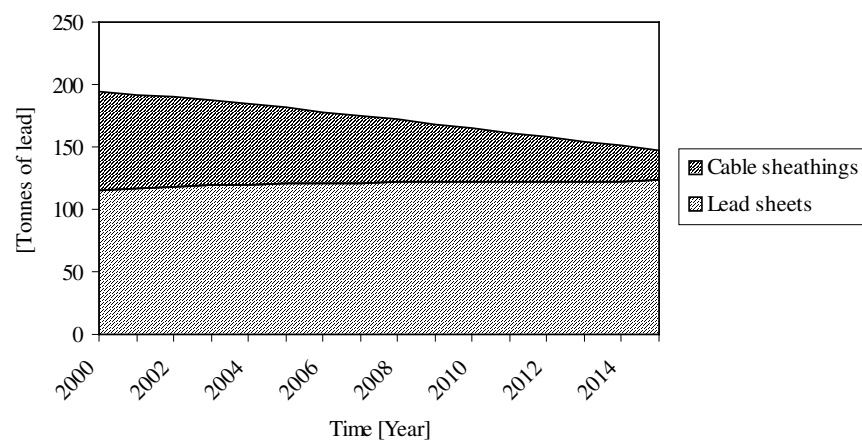
**Fig. 3:** Inflow of lead in different applications into the stock of products-in-use in the Netherlands, 1989-2025

### 5.4.2 Outflow of lead applications

Fig. 4a and 4b show the outflows out of the stock-in-use: the discarded applications in 4a and the emissions during use in 4b. As shown in Fig. 4a, the discarding of SLI batteries does not show a general trend. This was to be expected since the inflow is quite stable, and the life span of these batteries is short. However, discarding of traction and industrial batteries is expected to increase due to the increase of the inflow and their long life span. Although the inflow is leveling off, the amount of discarded lead sheet is expected to increase due to the extensive use of lead sheet in the past. Likewise, discarded cable sheathing is expected to keep increasing till the year 2010 due to its extensive use in the past. After 2010 it will start to decrease because it is phased out from some applications in 1970 and from almost all the remaining applications in 1990. Part of the discarded cable sheathings will not be removed from the soil, but will be left in the environment. The amount of discarded CRTs and non-battery vehicle applications is expected to increase. This is due to the extensive and still increasing use of computers and vehicles on the one hand, and to the delay as a result of the long life span of both computers and vehicles on the other hand.



**Fig. 4a:** Discarded outflow of lead applications from the stock of products-in-use, 2002-2025

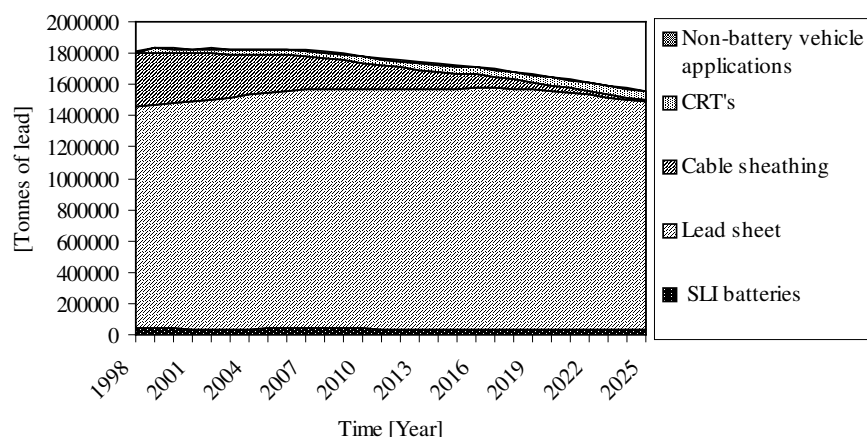


**Fig. 4b:** Emissions of lead applications during use, 2000-2015

Most of the lead applications in stock, such as batteries, CRTs and non-battery vehicle applications, have no emissions during their use phase. Therefore the emissions are mainly due to cable sheathing and lead sheet, which are exposed to the environment. As shown in Fig. 4b, emissions from lead sheet are expected to increase in future due to the expected increase of stock. However, the emissions from cable sheathing stock are expected to decrease slowly over time, as there is no fresh inflow in this stock while part of old stock is being collected and recycled. The remaining amount of cable sheathing in soil is quite high due to the low collection rate and the fact that lead sheathing has a relatively low commercial value. We assumed that 75% of the total amount of cable sheathing in the soil will be taken out. Nevertheless the contribution of cable sheathing to the lead emissions to the environment will remain rather high. The total emissions from the stock are expected to decline. This, however, does not mean that the total lead emissions will decrease. It should be kept in mind that there are other lead emissions to the environment not originating from the stock of products-in-use, especially related to agriculture and to incineration of fossil fuels.

### 5.4.3 Stocks of lead applications

The future development of the stock of lead is shown in Fig. 5. It is clear that lead sheet will dominate the stock-in-use for a long time to come due to the extensive use of lead sheet in the past and its long life span. The stock of SLI batteries is expected to decrease between 2000 and 2011 and will stabilize after 2012. The stock of CRTs is increasing due to the current extensive and increasing use and the relatively long life span. The stock of cable sheathings is decreasing and might be finished by the year 2025. There is no new inflow because cable sheathing is phased out. Most of the stock will become waste and will be partly recycled. The rest will remain in the environment, causing emissions for a long time to come. The stock of non-battery applications is invisible in Fig. 5 due to the fact that the stock of non-battery vehicle applications is and will remain relatively small.



**Fig. 5:** Stock of lead in several products-in-use in the Netherlands, 1998-2025

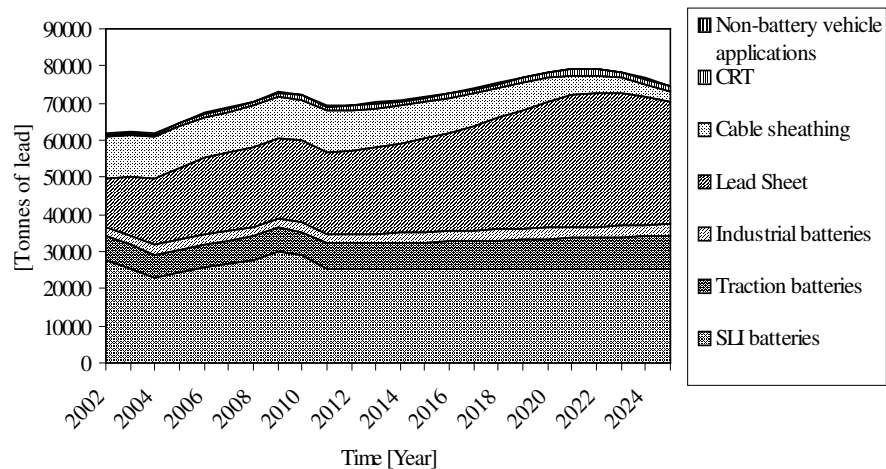
#### 5.4.4 Waste streams of lead applications

By far the largest fraction of the waste stream of lead is recycled. At present, the largest contribution to lead recycling is made by SLI batteries. In future, lead sheet is expected to be the largest contributor: the outflow of SLI batteries is expected to stabilize whereas the outflow of lead sheet will increase. Smaller contributions are made by other batteries: the recycling fraction is equally high or even higher, but the lead flow to these applications is smaller.

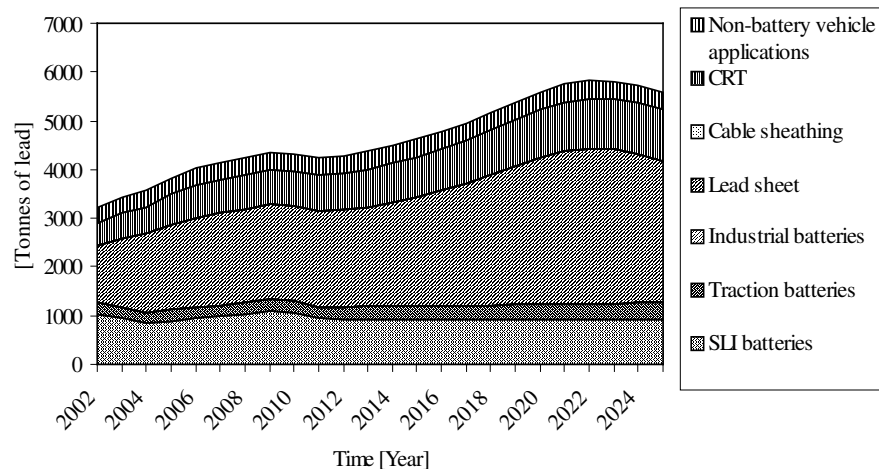
The largest flows to landfill and incineration are related to lead sheet, SLI batteries, and CRTs. This can be explained by the intensive use of both lead sheets and SLI batteries in the past and present: the recycling fraction for these applications is quite high, but the amounts are so large that the small percentage of final waste from these applications still amounts to a large quantity compared to others. The flow of waste CRTs has a low recycling fraction. The future flows of CRTs to landfill and incineration is expected to increase and by 2025 will cause almost 20% of the total lead flow to landfills. Flows to incineration and flows to landfill show a rather similar pattern. Only the contribution of lead sheet is different. A larger part of the discarded lead sheet will end up at landfill together with demolition waste, leaving only a very small fraction to be incinerated. The flows of the non-battery vehicle applications to landfill and incineration are relatively high compared to their throughput. This high contribution to the final waste stream is mainly due to low recycling fraction of these applications. The flow of the non-battery vehicle applications is invisible in Fig. 6a due to their relatively small outflow and low recycling fraction. Fig. 6a shows recycled flows of lead applications and 6 b, and c show total waste flows to landfills and incinerators.

#### 5.4.5 Future total lead inflow, outflow, stock and waste streams

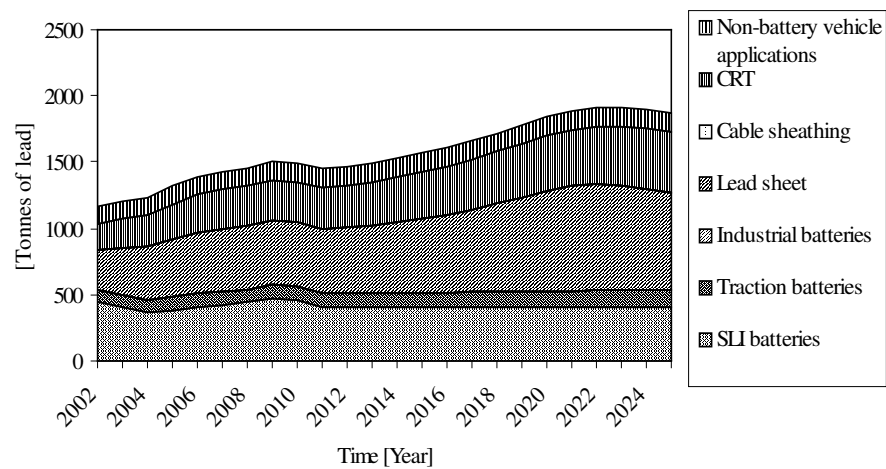
Fig. 7 shows the total inflow of lead into the stock of products-in-use and the total outflow of lead with discarded products. A remarkable development is that the outflow is larger than the inflow from 2002 onwards. This implies that the stock of lead in products is no longer a sink, but has become a source of lead. Due to the magnitude of the stock (Fig. 5), it can be expected that lead will be coming out of the stock for a long time, even in the case that lead applications would be phased out altogether. This is relevant information for waste management.



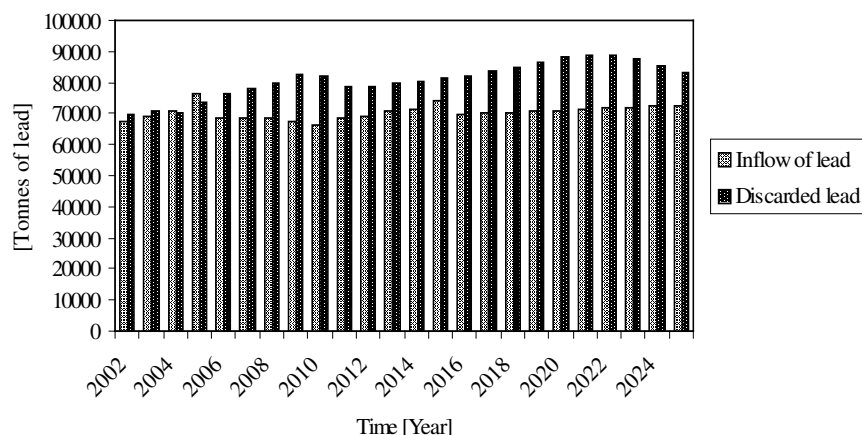
**Fig. 6a:** Flow of discarded lead to be recycled, 2002-2025



**Fig. 6b:** Flow of discarded lead to Landfill, 2002-2025



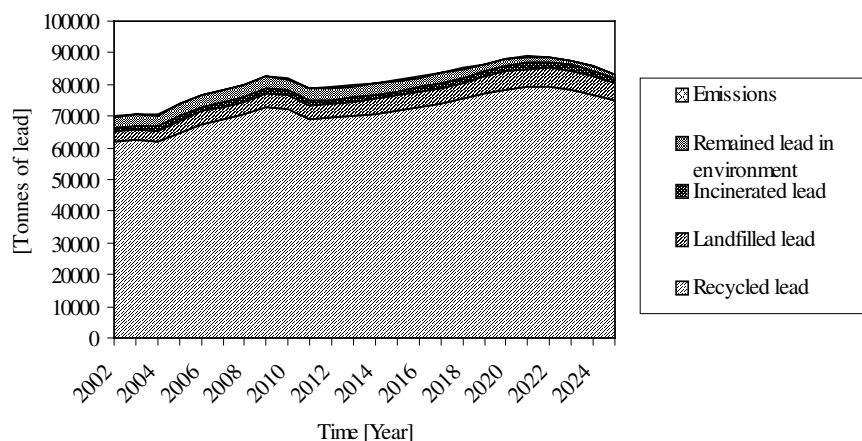
**Fig. 6c:** Flow of discarded lead to be incinerated, 2002-2025



**Fig. 7:** The total inflow of lead into the stock of products-in-use and the total outflow of lead with discarded products, 2002-2025

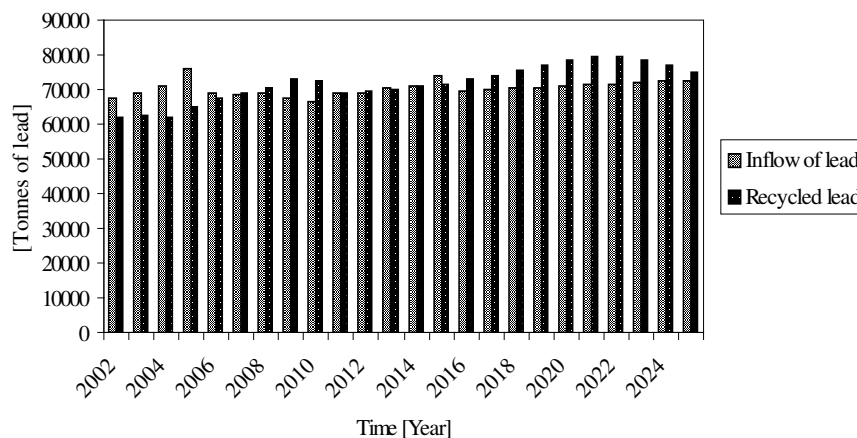
Although most of the lead applications are recycled (88% of the discarded stream), the amount ending up at landfill sites and incineration plants is still considerable. The percentage of landfill and incineration is even expected to increase slightly. Moreover, there is a significant amount of lead that remains in the environment in old cable sheathing. The remaining amount in soil, which will be almost 5.2% in 2002 will decrease to 4% in 2015. This hibernating stock will still cause diffusive emissions. The expectations for future recycling, landfill, incineration and emissions of lead, as well as the lead remaining in the environment, are shown in Fig. 8.

As stated before, by far the largest part of the lead outflow is recycled. This may have consequences for the future. Fig. 9 shows the future demand for lead applications and the availability of secondary lead.



**Fig. 8:** Recycling, landfill, incineration and emissions of lead and lead remaining in the environment, 2002-2025





**Fig. 9:** Future demand for lead and the availability of secondary lead, 2002-2025

It is clear that from 2002 to 2006, the demand for lead will be higher than what could be available from recycling. After 2006, the amount of lead to be recycled is expected to exceed the lead demand. This implies that after 2006 the total Dutch demand for lead could be met completely by the generated secondary lead. The dynamics of the production of secondary materials, however, is not confined to one country. The generated waste could be processed outside the studied geographical region and the demand could be met by importing refined lead or lead containing products. Since the analysis is limited to the Dutch economy, which is very open, the possibility that lead available for recycling could exceed its demand need not have large implications. However, when a similar pattern can be found in other countries as well or detected on a larger scale, this would mean that the supply of lead could outgrow the demand. This could have a number of implications. One implication could be a decrease in the lead price. Normally this would lead to an increase in the use, but since lead applications are subject to regulation this might not be so straightforward. On the other hand, it may lead to a decrease in the production of secondary lead, since recycling processes may become less profitable. In turn, this might lead to larger amounts of lead being dumped at landfill sites or being incinerated. This again could lead to larger emissions to the environment.

## 5.5 Discussion and conclusions

The lead model presented in this chapter is a dynamic substance stock model that combines physical and economic elements. By combining physical and economic elements into one model, the limitation of the existing economic and material flow models can be bypassed and their strengths combined. The model operates at two levels: the product level and substance level. This has enabled us to overcome the difficulties of modelling the substance stock: often it is not possible to directly model the substance stock because it is built up out of large number of applications, each showing a different behavior in the economic system.

The model calculates the development of the lead stock over time by the inflow and outflow characteristics of the individual lead applications. For each application, the inflow in the past is modelled as a function of the development in certain socio-economic factors using regression analysis. These factors appear to be sufficient to describe the past inflow. The derived model for the past then is transferred to the future, based on expectations about the development in the socio-economic factors. For the future, however, some other variables such as substitution and technological development might be equally important. These are as yet not included. The forecasts therefore are only valid assuming that no unpredicted changes, such as the development of a completely new substitute, will occur.

The outflow out of the stock of products-in-use is basically determined by two physical processes: leaching and delay. The leaching outflow, emissions during the use of the product, is modelled as a fraction of the stock-in-use. The delay outflow of waste products is modelled as the inflow of some time ago. Two factors

play an important role in determining the accuracy of the outcome of the model, namely the emission factors and the life span. The emission factors are assumed to be constant and the life span is assumed to fit a Weibull distribution. In reality both are subject to changes. Moreover, the estimates of both parameters are rather uncertain.

The model estimates the end-of-life treatment in the future - recycling, landfilling and incineration - based on the assumption that the current distribution of the waste stream over the three destinations will remain the same. In reality, these streams are subject to changes because of policy, technical, or economic reasons. In general, lead flows in waste and emissions should not be treated as final figures for several reasons. First, waste streams contain lead flows from other sources as well, such as waste from mining and industry. Loops and cycles within the end-of-life treatment system make especially the figures for landfill quite uncertain. Second, the model quantifies only part of the emissions from the use phase, while other emission sources such as emissions from extraction, production and waste treatment processes are not included at all. The lead model includes most of the intentional applications of lead, which constitute the largest part of the societal lead use. However, some other important applications from an environmental point of view, such as lead in ammunition or in fertilizers, are not included. The picture of the emissions to the environment resulting from the stock model is therefore far from complete.

Despite the above mentioned limitations, the stock model provides relevant information for a substance management. The results of this model can be presented in different ways, depending on the policy issue at hand. For example, the contribution of the different applications to landfill or to diffusive emissions can be specified over time, which is useful information for a waste prevention or pollution prevention policy. Another example is the future estimate of what will become available for recycling. From the model calculations it follows that the amount of lead available for recycling will increase and may even become larger than the demand for lead in the near future. This means that at least in the Netherlands the demand will be more than covered by the supply of secondary lead only. To draw a general conclusion, however, the analysis should be made on a larger scale (regional or global) where import and export do not play a big role. If comparable developments can be detected on a larger scale level as well, this may have consequences for the future management of lead. On the one hand, the demand for lead drops due to phase out policies. On the other hand, the supply from secondary sources increases as a result of the past building up of stocks in society. Moreover, the supply from primary sources still continues and is expected to continue for other reasons besides the demand for lead. All this may have consequences for the lead price and thus also for the profitability of primary production as well as the recycling industry. Consequently, this might increase the landfill and incineration streams at the expense of recycling, and ultimately may lead to an increase in the emissions.

The stock model has proven to be applicable and has delivered interesting results that cannot be obtained in any other way. The next step is then to put the stock model as a central module into a general substance flow model. In that way, the picture can be completed and the full implications of the interaction of stocks and flows may become apparent.

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## **Chapter 6    Long Term Consequences of Non-intentional Flows of Substances: Modelling Non-intentional Flows of Lead in the Dutch Economic System and Evaluating Their Environmental Consequences \***

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### **Abstract**

Substances may enter the economy and the environment through both intentional and non-intention flows. These non-intentional flows, including the occurrence of substances as pollutants in mixed primary resources (metal ores, phosphate ores and fossil fuels) and their presence in re-used waste streams from intentional use may have environmental and economic consequences in terms of pollution and resource availability.

On the one hand, these non-intentional flows may cause pollution problems, for instance by being emitted to air, water and soil or leaching out from road beds and landfill sites when secondary materials are utilized or landfilled. On the other hand, these flows have the potential to be a secondary source of substances and, thus, a possible solution for an expected shortage in the availability of some substances.

This chapter aims to quantify and model the non-intentional flows of lead related to the mixed primary resources and waste streams from intentional use, to evaluate their long-term environmental consequences and compare these consequences to those of the intentional flows of lead.

To meet this aim the model combines all the sources of non-intentional flows of lead within one model, which also includes the intentional flows. The demand for both intentional and non-intentional applications of lead is modelled on the basis of socio-economic variables.

Application of the model shows that the non-intentional flows of lead related to waste streams associated with intentional use are decreasing over time, due to the increased attention given to waste management. However, as contaminants in mixed primary resources applications lead flows are increasing, as demand for these applications is increasing.

The main source of lead emissions is the production of other heavy metals. Although non-intentional inflows of lead constitute less than 10% of the total lead inflow into the economy, the emissions of lead to the air from non-intentional applications are equal those from the intentional applications. Non-intentional flows of lead presently contribute 75% of the total amount of lead going to landfill and this is expected to rise to almost 90% by 2025.

The model presented in this chapter is illustrated by lead, can also be applied to other non-intentional flows of heavy metals.

**Key words:** substance flow analysis, dynamic modelling, lead, non-intentional flows

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\* Originally, “Elshkaki, A., Van der Voet, E., Van Holderbeke, M., Timmermans, V. (Submitted)”.

## 6.1 Introduction

The chemical and physical properties of heavy metals, such as lead, zinc, cadmium, copper, germanium, gallium and others means that they have many useful and intentional applications within the economy. Non-intentional applications of these metals arise from their natural occurrence in fossil fuels, other metal ores and phosphate ores and, in addition, secondary flows of these metals result from the processing of waste flows of their intentional applications.

These non-intentional flows have consequences in terms of pollution problems and resource availability. The consequences of the intentional flows of these substances have been studied extensively and several policies have been implemented to minimize their negative impacts. Less attention has been given to the consequences of the non-intentional flows, especially to the long-term consequences. This chapter seeks to provide an in-depth analysis of the potential problems caused by the non-intentional flows of lead in the Dutch economy.

Lead is a highly toxic metal. The American EPA cites lead as one of the 17 most dangerous chemicals in terms of the threat it poses to human beings and the environment (Wu et al., 2004). Lead can cause behavioural problems, learning disabilities, and can be fatal to children who inhale or ingest it. Moreover, lead can be toxic to plants, diminishing their productivity or biomass, and eliminating some species (Singh et al., 1997, Xiong, 1997 and Patra et al., 2004). Due to extensive use in the past, large stocks of lead have been built up in the economy and environmental concentrations may still be rising due to continuing emissions.

Several measures have been taken to reduce the negative impacts of lead. These include end of pipe technologies, stimulating recycling and phasing out some applications of lead, such as in water pipes, paint and gasoline. A recent EU directive prevents member states from allowing new electrical and electronic equipments containing lead, mercury, cadmium, chromium VI, and PBB or PBDE to be put on the market (Wu et al., 2004). Such measures have been effective in reducing emissions of lead to the environment, reducing human exposure and the subsequent health effects of the intentional applications of lead. However, despite effective management of these intentional applications, lead may still threaten human health through indirect routes of non-intentional flows. For example, lead enters the agricultural chain via phosphate fertilizer and accumulates there, leading to significant concentrations in manure. The processing of metal ores and the use of fossil fuels leads to emissions of lead to the environment, which may end up in waste streams. Part of this waste is landfilled and part is used as fly ash, bottom ash and slag in construction materials. In addition to direct emissions of lead to the air, water and soil, the accumulated lead in roads, buildings, agricultural soil and landfill sites may leach to the soil or ground water.

Thus, the environmental consequences of non-intentional flows of lead stem from different sources, which might develop differently in the future. For example, the flows of lead in the re-used waste stream from intentional use might decrease in the future due to policies aimed at reducing lead applications, or through increased recycling. On the other hand, flows of lead in fossil fuels, fertilizer or other metals may continue to rise as long as the demand for these applications is increasing.

The aim of this chapter is to evaluate the long-term direct environmental consequences of the non-intentional flows of lead, compare these with the consequences of the intentional flows of lead. In meeting this aim a dynamic model for non-intentional flows and stocks of lead is developed.

The accumulated secondary flows in roads and buildings can also be seen as secondary sources of lead. The availability of lead in the utilized and landfilled secondary materials (fly ash, bottom ash and slag) generated from the production of other heavy metals, electricity production from coal and the incineration of intentional applications of lead and of the accumulation of lead in buildings, roads and landfill sites will be discussed in the subsequent chapter.

To evaluate the long-term consequences of non-intentional flows of lead and other substances, the sources of these flows need to be combined and the factors determining their long-term development should be identified. Both economic factors related to supply and demand and technological factors describing process efficiency need to be included in the model.

The developed model combines functions that describe the long-term development of the main sources of non-intentional flows of lead (electricity production, production of other heavy metal, oil production and fertilizer use), based on statistical approaches and scenarios that describe the demand as a function of socio-economic variables such as GDP, population, price and other specific variables for each application (Burney, 1995, Ranjan and Jain, 1999, Mohamed and Bodger, 2004, Roberts, 1996, Moore and Tilton, 1996, Crompton, 2000, Mergos and Stoforos, 1997 and Bouwman and Hoek, 1997) and technological

factors describe process efficiency, with specific detailed models for the intentional applications of lead (Elshkaki et al., 2004).

This chapter is structured as follows. Section 2 outlines the methodology used in modelling non-intentional flows of lead in the economy and the environment. Section 3 quantifies the model's relations. Section 4 contains the results of the model's calculations and section 5 is dedicated to discussions and conclusions.

## 6.2 Methodology

### 6.2.1 General set up of the model

The core of the model used is based upon Substance Flow Analysis (SFA). SFA is widely used in the study of both pollution and resources. It is based on the materials balance principle, which enables different types of analysis. Substance flow accounts can be used to identify major flows and accumulations and to spot trends. Static models can be used to identify causes of pollution problems and assess the effectiveness of contra-measures (Van der Voet, 1996, Bringezu et al., 1997 and Bauer et al., 1997). Dynamic models allow for the analysis of the long-term development of stocks and flows, of forecasts of future emissions and waste streams from the stocks built-up within society and the inclusion of loops and cycles within the system (Kleijn et al., 2000 and Elshkaki et al., 2004). As such they can provide a relevant input for strategic environmental policy planning. In addition, SFA has proved to be a particularly suitable tool to spot the non-intentional flows: the occurrence of a substance as a trace contaminant in materials derived from fossil fuels, phosphate rock etc. (Guinée et al., 1999). This section presents the general set up of the dynamic SFA model for non-intentional flows of lead.

The non-intentional flows of lead in the economic and environmental systems are partly related to the waste streams of the intentional applications of lead and partly to the applications of mixed primary resources. The sources of non-intentional flows of lead are shown in Fig. 1.

#### *Input of lead from mixed primary resources containing lead as a contaminant*

The inflows of lead into the production of electricity, oil, and other heavy metals and its inflow into agricultural soil through its natural occurrence in ores and fossil fuels are determined by the demand these applications and the content of lead in the ores and fossil fuels.

The model uses a general function (Eq. 1) to describe the past development in the demand for electricity, oil, heavy metals, and phosphate fertilizers. The same function is used for the future with an assumption about the future development in the explanatory variables.

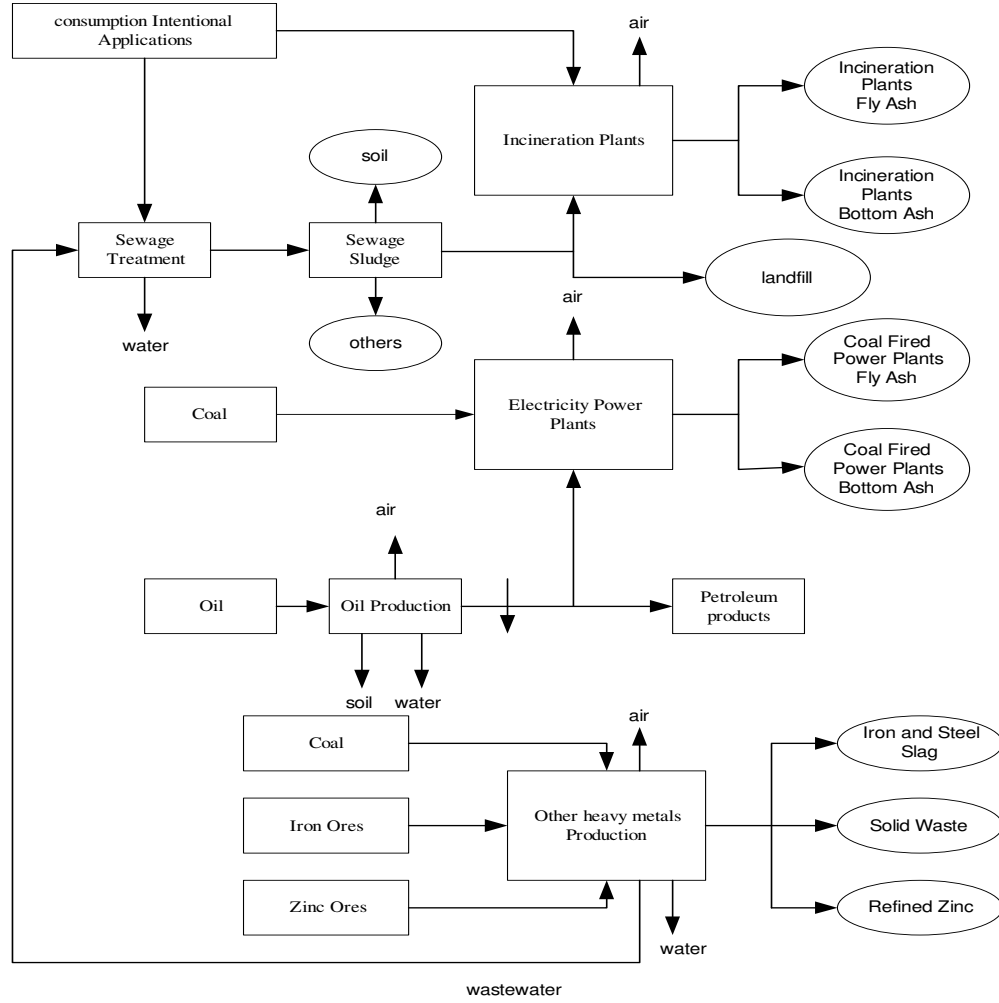
$$Y(t) = \beta_0 + \sum_{i=1}^n \beta_i X_i(t) + \varepsilon(t) \quad (1)$$

$Y(t)$  is the production of electricity, other heavy metals, oil and fertilizer use at time  $t$ ,  $X_i$ 's are the socio-economic variables at time  $(t)$ ,  $\beta$ 's are the model parameters and  $\varepsilon(t)$  is the model error.

An alternative, especially relevant when insufficient data are available or a discontinuity is expected is the use of scenarios. Here, the input of lead is modelled based on the amount of lead per ton of produced metal, per kwh electricity produced, and per ton of phosphate fertilizers used, as given by Eq. 2.

$$F_{L,Y}^{in}(t) = Y(t) \cdot L_x \quad (2)$$

where  $F_{L,Y}^{in}(t)$  is the inflow of lead at time  $t$ , and  $L_x$  is the amount of lead



**Fig. 1:** Non-intentional flows of lead in the economy and the environment

### *Input of lead arising from the waste streams from lead intentional use*

The inflows of lead into the economy through emissions from intentional applications during their use phase and the processing of their waste streams are determined by the demand for lead in intentional applications, their life span, the emissions factors and the waste management of discarded products.

The input of lead into sewage treatment plants originates from emissions of lead during the use phase of lead sheets, the production of other heavy metals and the consumption of food and animal products, as given by Eq. 3.

$$F_{ST}^{in}(t) = F_{CE,ST}^{out}(t) + F_{OHM,ST}^{out}(t) + F_{CFAP,ST}^{out}(t) \quad (3)$$

where  $F_{ST}^{in}(t)$  is the inflow of lead into sewage treatment plants at time  $t$ ,  $F_{CE,ST}^{out}(t)$  is the flow of lead originating from emissions during the use phase at time  $t$ ,  $F_{OHM,ST}^{out}(t)$  is the flow of lead originating from the production of other heavy metals, and  $F_{CFAP,ST}^{out}(t)$  is the flow of lead originating from consumption of food and animal products at time  $t$ .

The inputs of lead to sewage treatment plants from the use phase of lead sheets is estimated as a fraction of the emissions of lead during the use phase, as given by Eq. 4. Emissions of lead during the use of lead sheet are estimated as a fraction of the stock-in-use of lead sheet, as given by Eq. 5 (see Elshkaki et al., 2004).



$$F^{out}_{CE,ST}(t) = C_1 \cdot F^{out}_{C,E}(t) \quad (4)$$

$$F^{out}_{C,E}(t) = C \cdot S(t) \quad (5)$$

where  $F^{out}_{C,E}(t)$  is the outflow due to emissions at time  $t$ ,  $C_1$  is the fraction that determines the amount of lead ending up in sewage treatment,  $C$  is the emission factor and  $S(t)$  is the stock at time  $t$ .

The inflow of lead from the consumption of food and animal products is estimated from the amount of lead taken up from the agricultural soil by food and fodder. The uptake of lead by food and fodder is estimated as a fraction of the lead stock in the agricultural soil.

The inflow of lead from the production of other heavy metals is estimated as a fraction of the inflow of lead through iron ores and coal used in steel production, as given by Eq. 12.

The input of lead into incineration plants originating from the waste stream of lead containing products discarded from the stock-in-use and that part of the produced sewage sludge that is incinerated as given by Eq. 6. The input from sewage sludge is discussed in (2.6.3).

$$F^{in}_{inc}(t) = \sum_{i=1}^n F^{in}_{inc,DC,i}(t) + F^{in}_{inc,SS}(t) \quad (6)$$

where  $F^{in}_{inc}(t)$  is the inflow of lead into incineration plants,  $F^{in}_{inc,DC,i}(t)$  is the inflow of lead into incineration plants originating from discarded product  $i$  at time  $t$ , and  $F^{in}_{inc,SS}(t)$  is the inflow of lead into incineration plants originating from incinerated sludge at time  $t$ .

The future inflow of lead into incineration processes from the discarded outflow of the stock-in-use is estimated from assumptions for the distribution over incineration, landfill and recycling.

The incinerated flow of lead out of the discarded outflow of the different applications of lead is estimated as a fraction of the total amount of the substance going to be incinerated and landfilled, as given by Eq. 7.

$$F^{in}_{inc,DC,i}(t) = \alpha_{1,i}(t) \cdot F^{in}_{inc,land,i}(t) \quad (7)$$

where  $F^{in}_{inc,land,i}(t)$  is the amount of lead to be incinerated and landfilled at time  $t$ .

The total amount of lead to be incinerated and landfilled is estimated as the difference between the total discarded outflow and the flow collected for recycling as given by Eq. 8.

$$F^{in}_{inc,land,i}(t) = F^{out}_{C,D,i}(t) - F^{in}_{SC,i}(t) \quad (8)$$

where  $F^{out}_{C,D,i}(t)$  is the total discarded outflow from the stock-in-use of product  $i$  at time  $t$  and  $F^{in}_{SC,i}(t)$  is the scrap of product  $i$  collected for recycling at time  $t$ .

The collected flow for recycling is estimated as a fraction of the discarded outflow, as given by Eq. 9. The model uses a general function (Eq. 10) to describe the collection rate (CR), whose fit is based on past trend data for some applications, such as lead sheet. For other applications, assumptions are made about future collection rates.

$$F_{SC,i}^{in}(t) = CR_i(t) \cdot F_{C,D,i}^{out}(t) \quad (9)$$

$$CR_i(t) = \beta_0 + \sum_{i=1}^n \beta_i X_i(t) + \varepsilon(t) \quad (10)$$

The discarded outflow from the stock-in-use is estimated as the inflow at a given point in the past as given by Eq. 11 (see Elshkaki et al., 2004).

$$F_{C,D,i}^{out}(t) = F_{C,i}^{in}(t - L_{U,i}) - \sum_{i=1}^L C_i \cdot F_{C,i}^{in}(t - L_{U,i}) \cdot (1 - C_i)^{i-1} \quad (11)$$

where  $F_{C,D,i}^{out}(t)$  is the outflow due to the delay mechanism at time  $t$ ,  $C_i$  is the emission factor of product  $i$  and  $L_{U,i}$  is the life span of product  $i$  in use.

### ***Output of lead from different processes***

Outflows of lead from the production processes of oil, electricity and other heavy metals and incineration processes are determined mainly by technical factors. Lead flows associated with disposal routes of sewage sludge are determined mainly by policy aspects. These outflows are modelled as a fraction of the input, as given by Eq. 12. Mass balance is enforced by modelling one flow per process as a balancing item, in this case landfill.

$$F_{L,x}^{out}(t) = \alpha_x(t) \cdot F_{L,y}^{in}(t) \quad (12)$$

where  $F_{L,x}^{out}(t)$  is the outflow of lead to a specific destination at time  $t$ ,  $\alpha_x(t)$  represents the emissions factor, the partitioning of lead between fly and bottom ashes, and the different disposal routes of sewage sludge at time  $t$ .

Emissions factors are mainly determined by technological development. These can be assumed either to be constant or to change overtime and are modelled by either linear or exponential functions. Data for some of the emissions factors are available. The emissions data are fitted with a linear function, similar to the one given by Eq. 1, using time as a proxy of technological development and other time-related variables or they are fitted to an exponential function as given by Eq. 13.

$$\alpha_x(t) = \beta_0 \cdot e^{\beta_1 \cdot t} \quad (13)$$

The partitioning of lead between bottom ash and fly ash during incineration processes and electricity production is determined by technical factors (Hasselriis and Licata, 1996, Sandelin et al., 1999 and Sandelin and Backman, 2001). In the model the partitioning of lead is estimated, based on different sources, and is assumed to be constant.

The disposal routes of sewage sludge are determined mainly by policy aspects. They can be assumed constant, with the most recent values being used, or they can be assumed to change over time and modelled based on Eq. 1. Time can be used as a proxy of the policy aspects and other time-related variables.

## **6.2.2 The production of electricity**

### ***Input of lead into the production of electricity***

Electricity is generated from different sources such as coal, oil, natural gas, nuclear and others. The inflows of lead into the production of electricity are mainly due to the use of coal and heavy oil. The lead inflow is

estimated from the demand for electricity, the amount of coal and oil used in electricity production and the lead content in coal and oil.

Data on past electricity production in the Netherlands are available (CBS, 2003). For the future, a general function (Eq. 1) is used to describe electricity production, which is fitted based on past trend data using regression analysis. Electricity price, GDP, per capita GDP, and population size are the primary determinants of demand for electricity.

The amounts of coal and oil used in electricity production can be estimated either by using Eq. 1 and the factors determining the use of different sources, such as the price of different fuels, technology development and policy, or by using developed scenarios.

The input of lead from coal ( $L_x$  in Eq. 2) is estimated based on the total inflow of lead due to the use of coal in electricity production in 1990 (Annema et al., 1995) and the electricity produced from coal in the same year (CBS, 2003).

Data on the amount of lead related to the use of oil was difficult to find, therefore the outflows of lead are taken as being directly related to the production of electricity from oil, which is better known.

### ***Output of lead from the production of electricity***

The outflows of lead from the production of electricity from coal (lead emissions to air, lead in fly ash and lead in bottom ash) are estimated as fractions of the total input of lead into coal fired power plants as given by Eq. 12. These factors are estimated from work by Sandelin et al., (1999) and Sandelin and Backman (2001). The only flow related to the use of oil in electricity production is the lead emitted to the air, which is estimated as a fraction of electricity produced from oil. The factor is estimated using CMLCA software (Heijungs, 2000).

## **6.2.3 The production of other heavy metals**

### ***Input of lead into the production of other heavy metals***

The inflow of lead into the production of other heavy metals originates from the ores of zinc and iron and the coal used in steel production. The inflow of lead is estimated based on the amounts of zinc, iron and steel produced and the lead content in these ores and in coal.

Data on the past production of zinc, iron and steel are all available (USGS, 1980-1990, British Geological Survey, 1988-2000 and Metallgesellschaft Aktiengesellschaft, 1990). For the future, a general function (Eq. 1) is used to describe the production of these metals, which is fitted based on past trend data using regression analysis. The prices of these metals, GDP, per capita GDP, population and world demand are the primary determinants of the production of these metals.

The input of lead from zinc and iron ores ( $L_x$  in Eq. 2) is estimated from the total input of lead through iron and zinc ores in 1990 (Annema et al., 1995), lead in zinc concentrates, pre-refined zinc and refined zinc (Ayres et al. 2003) and the amount of zinc and iron produced in the NL in 1990. The input of lead due to the use of coal ( $L_x$  in Eq. 2) is estimated based on the total input of lead from coal in 1990 (Annema et al., 1995) and the amount of steel produced in the NL in 1990.

### ***Output of lead from the production of other heavy metals***

The outflows of lead from the production of other heavy metals are in the form of emissions of lead to air and water, the flow of lead to sewage treatment plants, the lead remaining in iron and steel slag, in refined zinc, and in landfilled solid waste generated by all these production processes.

Data on the past emissions of lead to air and water during the production processes of iron and steel are available (VROM, 1990). These data are tested with linear and exponential functions as given by Eq. 1 and Eq. 13 for the best correlation of the emission factor ( $\alpha_x$  in Eq. 12) using time as the explanatory variable.

The outflows of lead in slag and wastewater from the production of iron and steel are estimated as fractions of the lead input through iron and coal, as given by Eq. 12. The outflow of lead in refined zinc from the production of zinc is estimated as a fraction of the input of lead through zinc, as given by Eq. 12. The factors are estimated based on the work of Annema et al. (1995) and assumed to be constant.

The outflow of lead in solid waste stream is estimated as the difference between the total input of lead into the production of other heavy metals and the other outflows.

### **6.2.4 The production of oil**

Data on the past inflow of lead into the Dutch economy from the production of refined oil was difficult to find. Therefore the outflows of lead are estimated directly, based on the production of refined oil. Data on the past production of refined oil are available (CBS, 2003). For the future, a general function (Eq. 1) is used to describe the production of refined oil, which is fitted based on past trend data using regression analysis. GDP, per capita GDP, and population are the primary determinants of oil production. The outflows of lead from the production of refined oil are emissions of lead to the air, water and soil. These outflows are estimated as fractions of the produced oil. The factors are estimated using CMLCA (Heijungs, 2000).

### **6.2.5 The use of phosphate fertilizers**

Lead occurs as a contaminant in chemical fertilizers, due to its natural existence in the ores from which these fertilizers are made, especially phosphate ores. The inflow of lead is estimated based on the use of fertilizers and the lead content of phosphate fertilizers. Data on the past consumption of phosphate fertilizers are available (FAO, 2003). For the future, a general function (Eq. 1) is used to describe the consumption of fertilizers, which is fitted based on past trend data using regression analysis. The use of fertilizers is determined by several factors, including economic growth, population growth, fertilizer prices, the price of agricultural products, the relative price of fertilizers with respect to the price of agricultural outputs, lagged agricultural output price and policy measures. The input of lead ( $L_x$  in Eq. 2) is estimated based on the use of phosphate fertilizers in the NL in 1990 (FAO, 2003) and the inflow of lead to agricultural soil through fertilizers in the same year (CBS, 1993).

### **6.2.6 Sewage treatment**

#### ***Estimation of the inflows of lead into sewage treatment plants***

The input of lead into sewage treatment plants originates mainly from emissions of lead during the use phase of lead sheets. Of these emissions, roughly 50% are emitted directly to the soil and the other 50% enter the sewage system. The other inputs of lead to the sewage system originate from the production of other heavy metals and the consumption of food and animal products.

#### ***Estimation of the outflow from sewage treatment plants***

The outflows of sewage treatment plants are sewage sludge and effluent. The input of lead into sewage treatment plants will end up in one of these two media, depending on the efficiency of the process. It is estimated that 80% of lead input into sewage treatment plants ends up in sewage sludge (Annema et al., 1995) and 20% in the effluent.

#### ***The disposal routes of sewage sludge***

Sewage sludge is disposed of in different manners. Some is used as a soil improver, some is incinerated and the remainder is landfilled. Data on the past disposal routes of sewage sludge are available (CBS, 2003). The future development in the disposal routes of sewage sludge can be estimated either by the general equation (Eq. 1) and the time as proxy time-related variables, or by assuming that the most recent values of different disposal routes are valid for the future.

## 6.2.7 Incineration processes

### *Input of lead into incineration plants*

The input of lead into incineration plants originates from the waste stream of products containing lead that have been discarded from the stock-in-use, together with the fraction of sewage sludge that is incinerated. Data on the past incinerated mixed solid waste and bottom and fly ash are available (VVAV, 2001). The lead content of bottom ash and fly ash is assumed to be equal to estimates made by Kosson et al. (1996). The future inflow of lead into incineration processes from the discarded outflow from the stock-in-use is estimated, based on Eqs. 7, 8, 9, 10, and 11. The input of lead into incineration processes from sewage sludge is discussed in 2.6.3.

### *Output of lead from the incineration plants*

The outflows of lead from incineration plants in bottom ash, fly ash and emissions from incineration process are estimated as fractions of the total inflow of lead into incineration plants, as given by Eq. 12. The partitioning of lead ( $\alpha_x$  in Eq. 12) amongst the incineration residues is estimated as 85% in the bottom ash and 15% in the fly and combined ash (Van der Sloot, 1996), with the lead content in bottom ash being 1500 mg lead/kg and 4000 mg lead/kg in the fly ash.

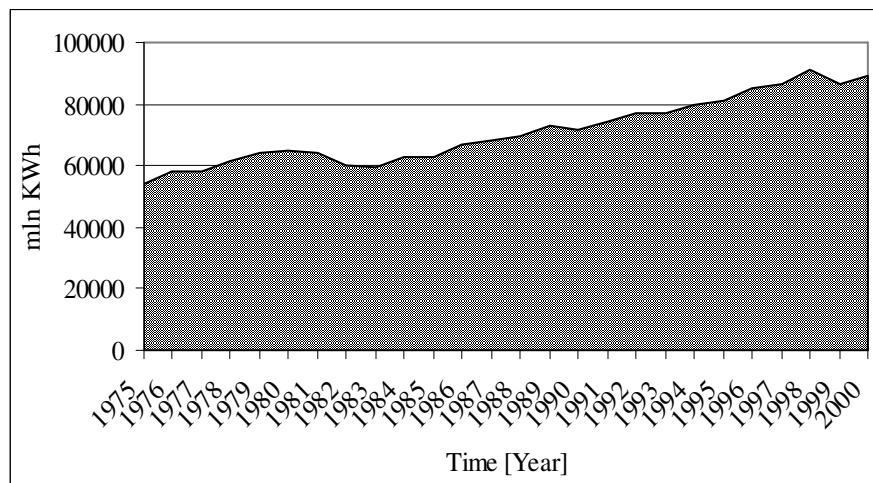
## 6.3 Quantification of model relations - Results of the analysis

### 6.3.1 The production of electricity

The total electricity produced in the NL between 1975 and 2000 (Fig. 2) (CBS, 2003) has been tested for correlation with all the expected influential explanatory variables such as the population size, GDP, per capita GDP, and electricity own price. The results are shown in table 1. The results indicate a positive correlation between all the tested variables and the production of electricity, significant at the 99% probability level. The coefficient of determination ( $R^2$ ) associated with the correlation is fairly high. The highest coefficient of determination ( $R^2=0.95$ ) is the one associated with population and GDP. On this basis the following equation is used to calculate total electricity production:

$$TEP(t) = -47018 + 0.00713 \cdot pop(t) + 5.4E - 9 \cdot GDP(t) \quad (14)$$

where  $TEP(t)$  is the total electricity production at time  $t$ .

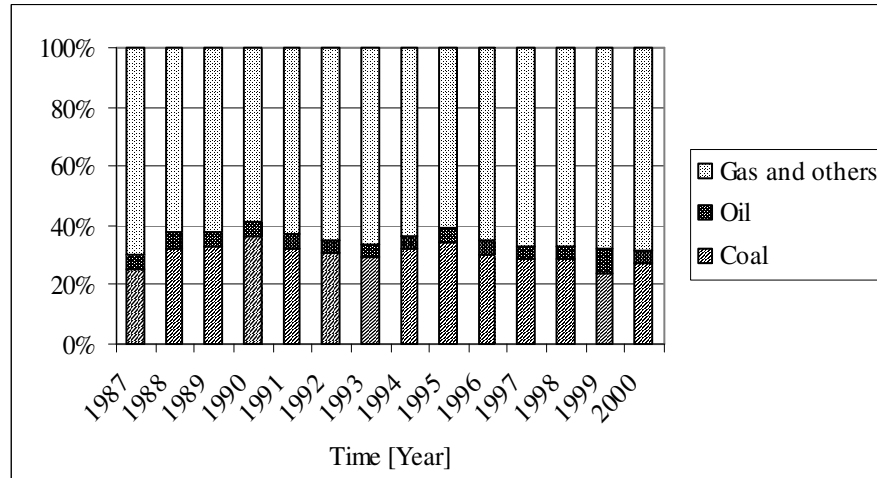


**Fig. 2:** Total electricity production in the NL 1975-2000

The share of the main sources used for electricity generation from 1987 through 2000 (Eurostat, 1987-2000) is shown in Fig. 3. The future share of the main sources in electricity generation is estimated from Eq. 1 and time is used as a proxy of all time-related variables. The following model relations are used to calculate the future share of coal and gas and other sources. The share of oil is estimated by Eq. 17.

**Table 1:** Analysis of the production of zinc, iron, steel, electricity, oil and fertilizer use in the Dutch economy

Variable	B <sub>0</sub> (t-value)	B <sub>1</sub> (t-value)	β <sub>2</sub> (t-value)	B <sub>3</sub> (t-value)	R <sup>2</sup>	F-statistics
<b>Zinc</b>						
Population	-87610(-1.6)	0.01947(5.5)			0.62	31.3
GDP	178998(28.2)	9.54E-9(4.2)			0.48	18.0
Per capita GDP	177161(25.7)	0.15521(4.1)			0.47	17.2
Price	175418(13.9)	25.2351(2.3)			0.22	05.5
Pop, GDP	-293577(1.8)	0.03478(3.0)	-8.87E-9(1.3)		0.65	17.3
GDP, price	169363(16.5)	8.29E-9(3.3)	11.3575(1.1)		0.52	09.9
Pop, price	-71204(1.3)	0.01768(4.6)	9.12402(1.1)		0.64	16.4
Pop, GDP, price	-293880(1.9)	0.03416(3.0)	-9.69E-9(1.5)	10.34(1.3)	0.68	12.6
<b>Iron</b>						
Population	-6.8E6(-2.5)	0.77(4.3)			0.49	18.6
GDP	3.78E6(13.8)	4.4E-7(4.5)			0.52	21.0
Per capita GDP	3.68E6(12.6)	7.3(4.6)			0.52	21.2
Price	1.09E6(0.6)	6730(2.1)			0.19	04.4
Pop, GDP	1.9E6(0.2)	0.13(0.2)	3.7E-7(1.1)		0.52	10.0
GDP, price	2.53E6(1.7)	4E-7(3.7)	2359(0.9)		0.54	10.7
Pop, price	-6.6E6(-2.4)	0.73(3.3)	1192(0.4)		0.49	08.9
Pop, GDP, price	4.5E6(0.5)	-0.16(-0.2)	4.8E-7(1.3)	2727(0.8)	0.54	06.8
<b>Steel</b>						
Population	-6.14E6(-2.4)	0.78(4.7)			0.53	21.7
GDP	4.45E6(17.2)	4.4E-7(4.8)			0.54	23.1
Per capita GDP	4.36E6(15.5)	7.21(4.7)			0.54	22.3
Price	1.3E6(0.8)	7404(2.4)			0.24	06.1
Pop, GDP	741375(0.1)	0.27(0.47)	2.96E-7(0.9)		0.55	11.2
GDP, price	2.7E6(2.0)	3.86E-7(3.8)	3219(1.3)		0.58	12.7
Pop, price	-6.1E6(-2.4)	0.7(3.4)	2066(0.7)		0.54	10.8
Pop, GDP, price	4.06E6(0.5)	-0.11(-0.2)	4.38E-7(1.3)	3459(1.16)	0.58	08.0
<b>Electricity</b>						
Population	-156373(-12.3)	0.0154(17.9)			0.93	323.0
GDP	48170(36.5)	9.7E-9(19.0)			0.94	363.0
Per capita GDP	46208(29.8)	0.158(17.4)			0.92	302.0
Pop, GDP	-47018(-1.4)	0.00713(2.8)	5.413E-9(3.4)		0.95	236.0
<b>Oil production</b>						
Population	-125323(-5.9)	0.01173(8.4)			0.85	71.0
GDP	35547(18.6)	5.63E-9(8.9)			0.86	79.4
Per capita GDP	34286(16.5)	0.09212(8.7)			0.86	76.8
Pop, GDP	-29504(-0.4)	0.00472(0.9)	3.46E-9(1.44)		0.87	39.8
<b>Fertilizers</b>						
Population	272694(22.6)	-0.013(-15.5)			0.86	241
GDP	106568(62.4)	-1.2E-7(-14.9)			0.85	224
Per capita GDP	107936(62.4)	-1.93(-15.4)			0.86	237
Population G	47552(6.5)	0.351(5.5)			0.45	30
Price	174785(21.8)	-195(-11.0)			0.81	122
Time	114932(57.2)	-1386(-16.2)			0.87	263
Time, PopG	114075(16.4)	-1375(-11.2)	0.005(0.13)		0.87	128



**Fig. 3:** The share of different sources for electricity production in the past 1987-2000

$$GOSS(t) = -6.621 + 0.0036 \cdot t \quad (15)$$

$$CS(t) = 6.7203 - 0.0032 \cdot t \quad (16)$$

$$OS(t) = 1 - [GOSS(t) + CS(t)] \quad (17)$$

where  $GOSS(t)$  is the share of gas and other sources at time  $t$ ,  $CS(t)$  is the share of coal at time  $t$  and  $OS(t)$  is the share of oil at time  $t$ .

Alternatively, the future share of the main sources for generating electricity can be estimated using different scenarios. National Institute of Public Health and the Environment (RIVM) has developed four scenarios for the future use of different sources in electricity production for OECD Europe based on different economic, environmental and social assumptions (Image team, 2001). Two of these scenarios (A2 and B2) are used in the estimates of lead flows from using coal in electricity production and compared with the outcome of the model.

### 6.3.2 The production of other heavy metals

The amounts of refined zinc, iron and steel from 1980 through to 2000 (USGS, 1980, British Geological Survey, 1988-2000 and Metallgesellschaft Aktiengesellschaft, 1990) have been tested with the all expected influential explanatory variables, such as the population size, GDP, per capita GDP, and metals price. The results are shown in table 1.

The results indicate a positive correlation between the production of these metals and all the tested variables. The correlation between the tested variables and zinc, iron and steel production is significant at the 99% probability level. The coefficient of determination ( $R^2$ ) associated with the correlation is fairly high, with the exception of the correlation with the price. For zinc, the highest coefficient of determination ( $R^2=0.62$ ) occurs with population and, for iron and steel the highest coefficients of determination ( $R^2=0.52$  for iron,  $R^2=0.54$  for steel) occur with per capita GDP. When the variables are combined, the coefficients of determination do not change significantly from those associated with the population in the case of zinc and per capita GDP in the case of iron and steel. Therefore, the following models will be used to calculate the production of the three metals:

$$ZP(t) = -87610 + 0.01947 \cdot pop(t) \quad (18)$$

$$IP(t) = 3.68E6 + 7.3 \cdot GDP / C(t) \quad (19)$$

$$SP(t) = 4.36E6 + 7.21 \cdot GDP / C(t) \quad (20)$$

where  $ZP(t)$  is the production of zinc at time  $t$ ,  $IP(t)$  is the production of iron at time  $t$  and  $SP(t)$  is the production of steel at time  $t$ .

### 6.3.3 The production of oil

The production of refined oil in the NL between 1985 and 1998 (CBS, 2003) has been tested for correlation with all expected influential variables, such as the population size, GDP, and per capita GDP. The results are shown in table 1. The results indicate a positive correlation between all the tested variables and the production of oil, significant at the 99% probability level. The coefficient of determination ( $R^2$ ) associated with the correlation is fairly high. The highest coefficient of determination ( $R^2=0.86$ ) occurs with GDP and per capita GDP. When variables such as GDP and population were combined, the coefficient of determination does not change significantly from those associated with GDP or per capita GDP and both variables turn out to be insignificant. Therefore, the following model will be used to calculate oil production in the NL:

$$OP(t) = 35547 + 5.63E - 9 \cdot GDP(t) \quad (21)$$

where  $OP(t)$  is the production of oil at time  $t$ .

### 6.3.4 The use of phosphate fertilizers

The inflow of phosphate fertilizers into the Dutch economy between 1961 and 2000 (FAO, 2003) has been tested for correlation with all expected influential variables. The explanatory variables used in the analysis are population size, GDP, per capita GDP, agricultural output price, population growth and time as a proxy of the effect of other influential variables on the inflow of phosphate fertilizers. The analysis covers the period 1961 to 2000. The relation between the price and the inflow of phosphate fertilizer is analyzed from 1966 to 1995. The results are shown in table 1. It is clear from the analysis of the inflow that all the independent variables correlate negatively with the inflow, except population growth. This is to be expected because fertilizer use is declining and the variables are increasing. This means that it is difficult to explain developments in fertilizer use from variables such as GDP, population, per capita GDP or price. Instead, we use the time variable to model the inflow. Using time as the explanatory variable, the coefficient of determination ( $R^2$ ) associated with correlations is fairly high. The time variable correlates negatively with the inflow. This indicates that other factors have influenced the use of fertilizers in the NL and it is clear that policy has had a large influence on the decline in fertilizer use. Therefore, the following model will be used to calculate the future demand for phosphate fertilizers in the NL:

$$F_{fert}^{in}(t) = 114932 - 1386 \cdot t \quad (22)$$

where  $F_{fert}^{in}(t)$  is the inflow of fertilizers at time  $t$ .

The future use of fertilizer can be estimated using time as the explanatory variable since this can capture the influence of the policy on fertilizer use.

The linear function estimated by regression analysis gives a good fit for the past. However, for the future the same equation lead to a considerable reduction in the use of fertilizers. A scenario developed by RIVM (Egmond et al., 2001) shows that the use of phosphate fertilizer will be stabile in the future at 38 million kg p.a.. Therefore, this value is taken as the minimum value for the use of fertilizer in the model.

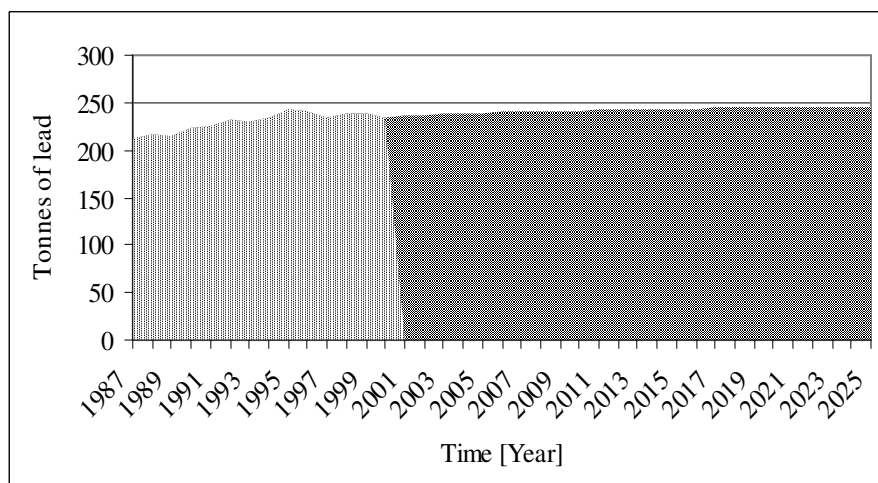


## 6.4 Results of the model

### 6.4.1 Non-intentional inflows of lead

#### *The production of electricity*

The input of lead through coal used in electricity production ( $L_x$  in Eq. 2) is given in table 2. The inflow of lead based on Eqs. 14, 16, and 2 and the value given in table 2 is shown in Fig. 4.



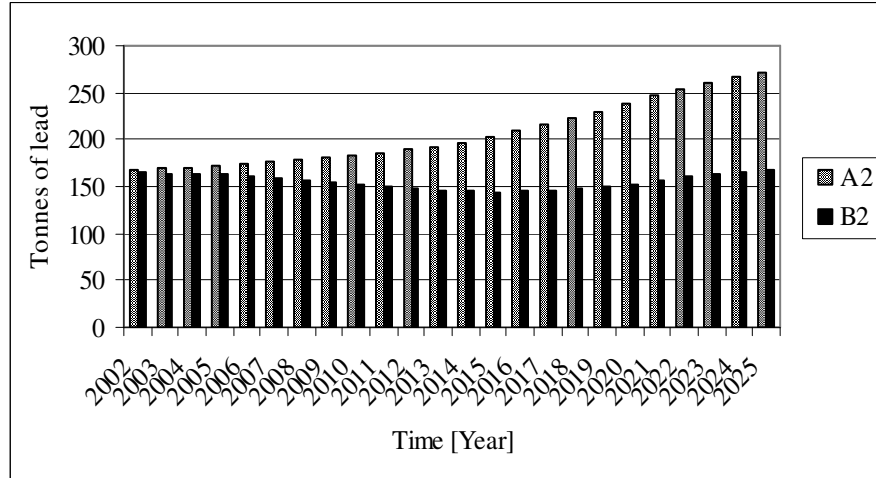
**Fig. 4:** The inflow of lead into the Dutch economy through the coal used in electricity production

As shown in Fig. 4, the non-intentional flow of lead from the production of electricity from coal is slowly increasing until 2017; and stabilizes thereafter. This is mainly due to the expected increase in the demand for electricity combined with the expected decrease in the use of coal in the generation of electricity.

**Table 2:** Lead content in different flows ( $L_x$  in Eq.2)

Flow	Lead content ( $L_x$ )
<b>Production of other heavy metals</b>	Kg of lead per ton of metal produced
Zinc	26.0
Iron	0.2
Coal	8.32 E-3
<b>Electricity production</b>	Kg of lead per mln kWh electricity produced
Coal	9.13
<b>Use of fertilizers</b>	Kg of lead per ton of phosphate fertilizers
Phosphate fertilizers	0.135

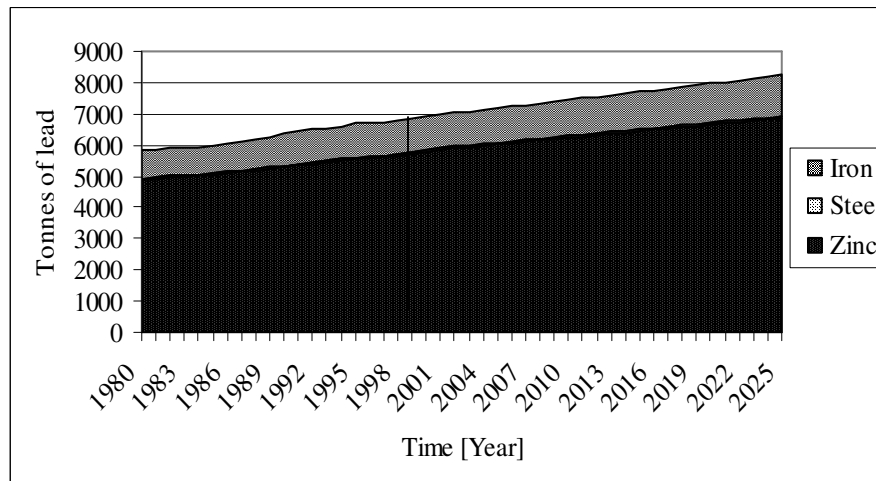
Fig. 5 shows the non-intentional flow of lead from the production of electricity from coal, based on two scenarios. Although the share of coal is decreasing, its use is increasing, due to the increase in electricity demand. The total use of coal in electricity production estimated based on A2 scenario is less than that estimated from the model to 2020, but more after that date. The estimated use of coal based on the B2 scenario is less than that estimated from the model.



**Fig. 5:** The inflow of lead through the coal used in electricity production based on two scenarios

### *The production of other heavy metals*

The inputs of lead through zinc, iron and steel ( $L_x$  in Eq. 2) are given in table 2. The past and future inflows of lead based on Eqs. 18, 19, 20, and 2 and the values given in table 2 are shown in Fig. 6.

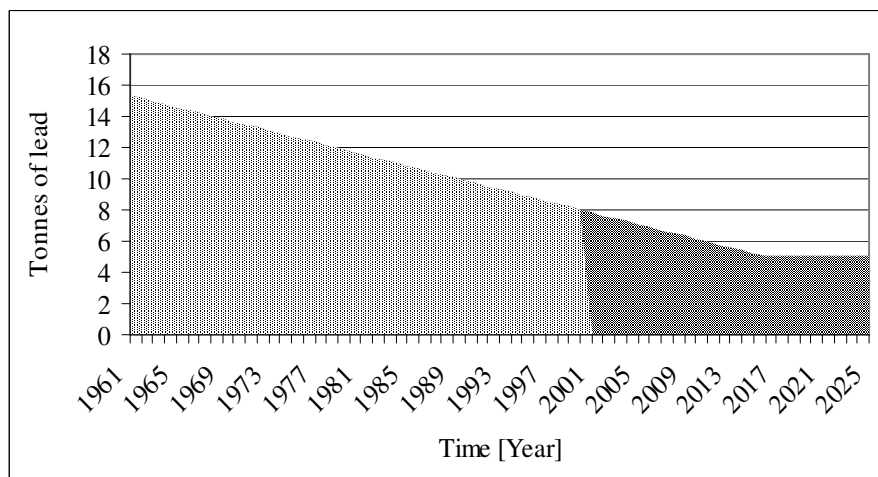


**Fig. 6:** The past and future inflow of lead in other metals

As shown in Fig. 6, the non-intentional flows of lead due to the production of zinc, iron and steel are increasing overtime. This is mainly due to the expected increase in the demand for these metals. Although the production of iron and steel in the Netherlands is greater than the production of zinc, the input of lead from zinc production is higher, due to the high content of lead in zinc ores.

### *The use of phosphate fertilizers*

The input of lead through phosphate fertilizers ( $L_x$  in Eq. 2) is given in table 2. The past and future inflow of lead through phosphate fertilizers based on Eq. 22 and the RIVM scenario and the value given in table 2 is shown in Fig. 7.

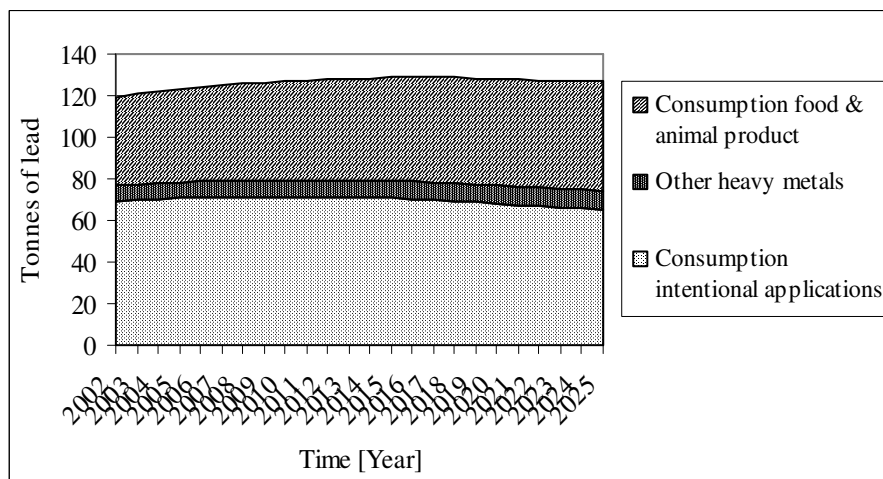


**Fig. 7:** The inflow of lead in the past and the future into Dutch agricultural soil

As shown in Fig. 7, the inflow of lead into agricultural soil from the use of phosphate fertilizers is decreasing overtime and is expected to stabilize in 2017 at 5.13 tonnes. This is mainly due to policy, which aims to reduce fertilizer use.

### ***Sewage treatment plants***

The input of lead into sewage treatment plants from different sources is shown in Fig. 8.

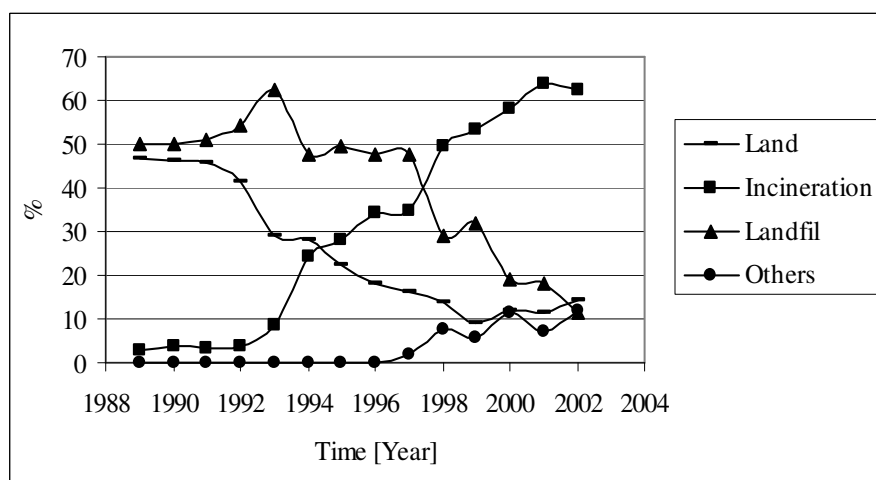


**Fig. 8:** The inputs of lead into sewage treatment plants

The main source of lead in sewage sludge is from emissions from the consumption of intentional lead applications. These are decreasing over time, due to the decrease in lead stocks in use. The second largest source of lead is the consumption of food and animal products, which is increasing over time due to the increase of lead inputs into agricultural soil and consequently its uptake in food and fodder. The third flow originates from the production of other heavy metals, which is increasing due to the increase in the production of iron and steel.

### ***The disposal routes of sewage sludge***

The disposal routes of sewage sludge in the past are shown in Fig. 9.



**Fig. 9:** Past disposal routes of sewage sludge

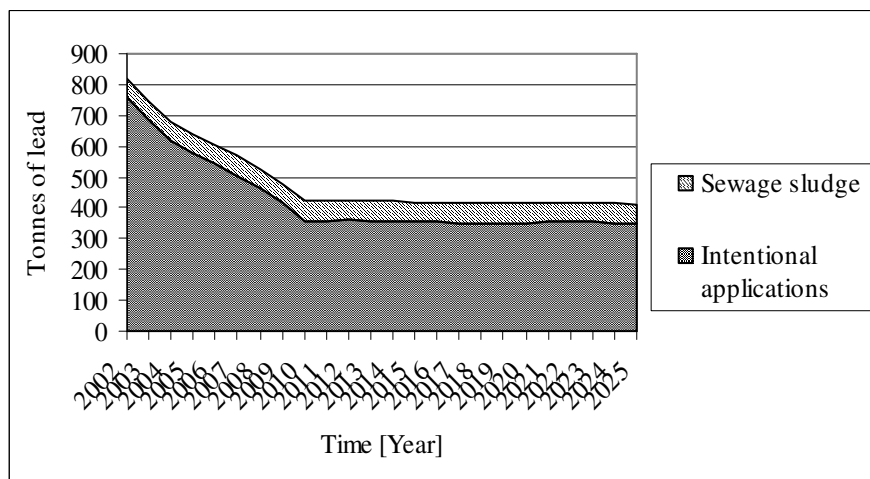
It is clear that the incineration of sewage sludge is increasing over time and the other disposal routes are decreasing. This is mainly due to the policy influences in the NL. Two future options for these different disposal routes are investigated. First, the values of different disposal options in the year 2001 are assumed to be constant in order to evaluate the current situation on the management of sewage sludge. The landfilled stream is assumed to be the difference between the total lead within sewage sludge and the lead in other disposal routes (incineration, land, others). Second, the incineration is modelled based on Eq. 1 with time being used as a proxy of time-related variables. If the current trend continues, the incineration of sewage sludge will reach 100% by the year 2009. If the current practice of sewage sludge management continues, 12% of lead in sewage sludge will end up in landfill sites and 62% of it will enter incineration plants. Due to the current management of incineration residues, about 15% of the lead entering incineration plants will also end up in the landfill sites, meaning that 27% of lead in sewage sludge will end up in landfill sites. If the current trend of increasing incineration of sewage sludge continues and reaches 100% in the year 2009, the landfilled lead, including the landfilled streams of bottom and fly ash will account for 23% of the total lead contained in sewage sludge.

### ***Incineration processes***

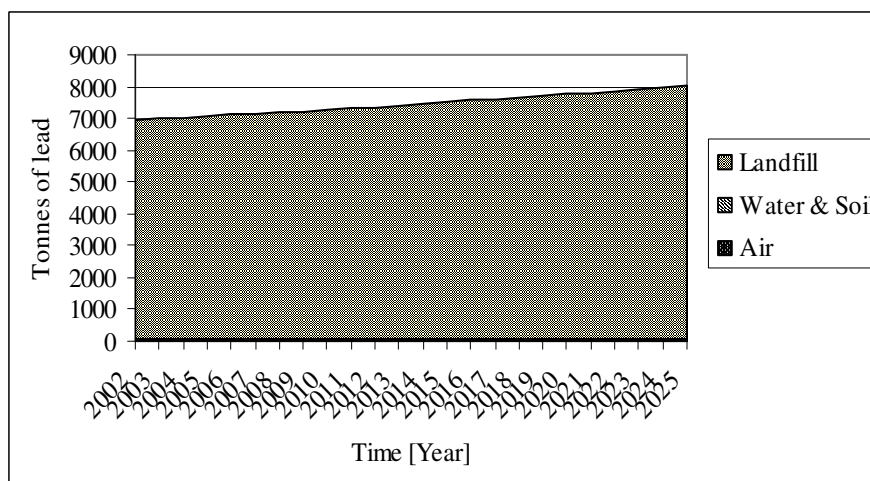
The input of lead into incineration plants from discarded applications and sewage sludge is shown in Fig. 10. By far the largest source is the outflow of discarded applications of lead out of the stock of products in use. This is decreasing over time, due to an increase in the recycling of intentional lead applications. The second largest flow is the stream of incinerated sewage sludge, which is increasing over time.

## **6.4.2 Non-intentional outflows of lead**

Some of the non-intentional outflows of lead, in particular those from the production of electricity, other heavy metals, refined oil, together with the flows from incineration plants and wastewater treatment plants, are released directly to the environment. Other outflows either enter new economic applications such as parts of the fly ash, bottom ash and slag or are sent to landfill sites. The total non-intentional outflows of lead to the air, water, soil and to landfill sites are shown in Fig. 11.



**Fig. 10:** The inputs of lead into incineration plants



**Fig. 11:** Non-intentional outflows of lead to air, water, soil and landfill sites

Sometimes, it is not clear where exactly to draw the border between the economy and environment. A landfill exists in the environment but is under human control. However, the choice of treating a landfill as part of the environment or of the economy does not make any difference in modelling terms or to the outcome of the SFA model. This is in contrast to, for example, LCA where the boundary between the technical system and the environment has to be drawn as one of the system boundaries (Guinée et al. 1993), as it determines what to call “emissions”). It is generally accepted that the emissions from landfill sites should be included in the inventory and therefore, that landfill sites should be included in the economic system (Heijungs et al. 1992 and Finnveden et al. 1995).

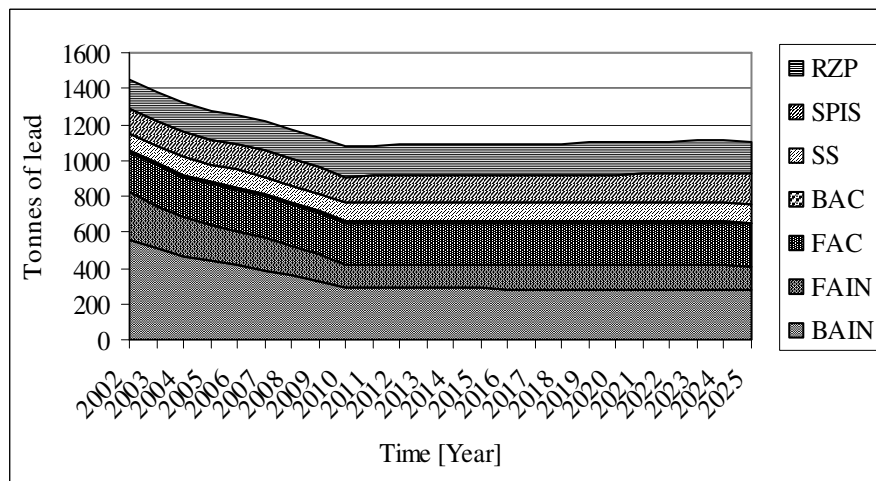
### ***Lead in secondary materials***

Table 3 shows the partitioning of lead to bottom ash and fly ash during the production of electricity from coal, the factors used to estimate lead outflows from the production of other heavy metals and the partitioning of lead to fly ash and bottom ash during incineration processes ( $\alpha_x$  in Eq. 12). Figure 12 shows the future outflows of lead in secondary materials based on the figures provided in Table 3 and Eq. 12. These lead outflows arising from the production of electricity from coal, of other heavy metals and from incineration plants. The flows in secondary materials are coded as follows: lead in fly ash and bottom ash

from electricity production (FAC and BAC respectively), lead in iron and steel slag (SPIS), lead in refined zinc (RZP) lead in the bottom ash and fly ash from incineration (BAIN and FAIN respectively) and lead in sewage sludge (SS).

**Table 3:** Factors used for different flows ( $\alpha_x$  in Eq. 12)

Flow	Factors ( $\alpha_x$ )
<b>Production of other heavy metals</b>	
Emissions of lead to air	$3E73\exp(-0.0863*t)$
Emissions of lead to water	$3E182\exp(-0.214*t)$
Lead in iron and steel slag	12.1%
Lead in wastewater	0.675%
Lead in refined zinc	2.7%
<b>Electricity production</b>	
Coal – emissions of lead to air	0.4%
Coal – lead in fly ash	95.6%
Coal – lead in bottom ash	4%
Oil – emissions of lead to air	0.128 kg of lead per TJ of produced electricity
<b>Oil production</b>	
Emissions of lead to air	1.65 E-4
Emissions of lead to water	3.38 E-4
Emissions of lead to soil	3.45E-5
<b>Sewage sludge disposal routes</b>	
Incineration	62%
Land	15%
Others	11%
<b>Incineration processes</b>	
Emissions of lead to air	0.07%
Lead in fly ash	31.93%
Lead in bottom ash	68%
<b>Landfilling</b>	
Fly ash generated from incineration	50%
Bottom ash generated from incineration	10%
Sewage sludge	27%



**Fig. 12:** Lead in secondary materials

Figure 12 shows that the total non-intentional flows of lead within secondary materials decreasing from 2002 to 2010 and slightly increasing thereafter. The initial decrease is largely due to the decreasing stream of lead in fly and bottom ash from incineration plants, which constitute the largest flows of lead in secondary materials. The outflows of lead generated from the production of electricity from coal will increase due to an increase electricity production. The outflows of lead in slag and refined zinc will increase due to increases in zinc production. Possible ways of utilizing these secondary flows will be discussed in more detail in the following chapter.

### ***Emissions of lead to the air***

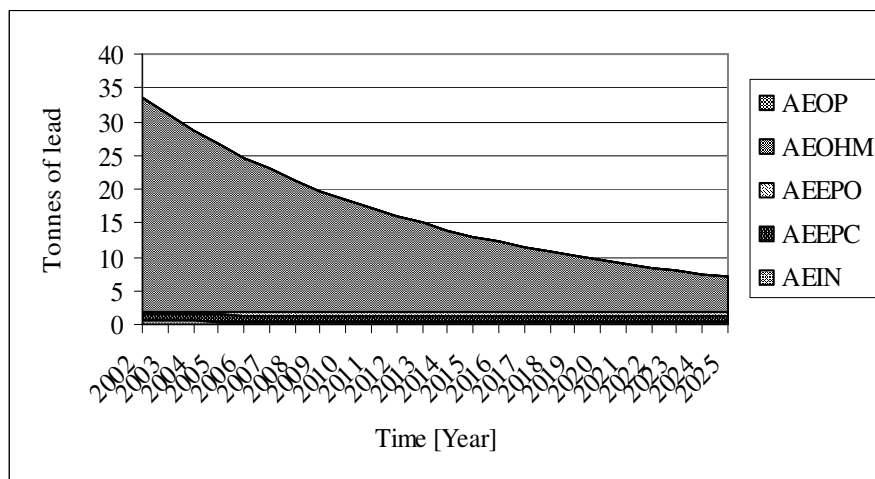
Air emission factors ( $\alpha_x$  in Eq. 12) are given in table 3. Based on these figures and Eq.12, Figure 13 shows future emissions of lead to the air from: coal and oil fired power plants (AEEPC and AEEPO respectively), the production of other heavy metals (AEOHM), oil refining (AEOP) and incineration plants (AEIN).

The Figure shows total emissions of lead to the air to be decreasing over time due to the decline in emissions from the production of other heavy metals, which is the largest source of lead emissions to the air from non-intentional sources. Although, the demand for these other heavy metals is increasing, emissions of lead from their production are decreasing due to the assumed reduction in emission factors.

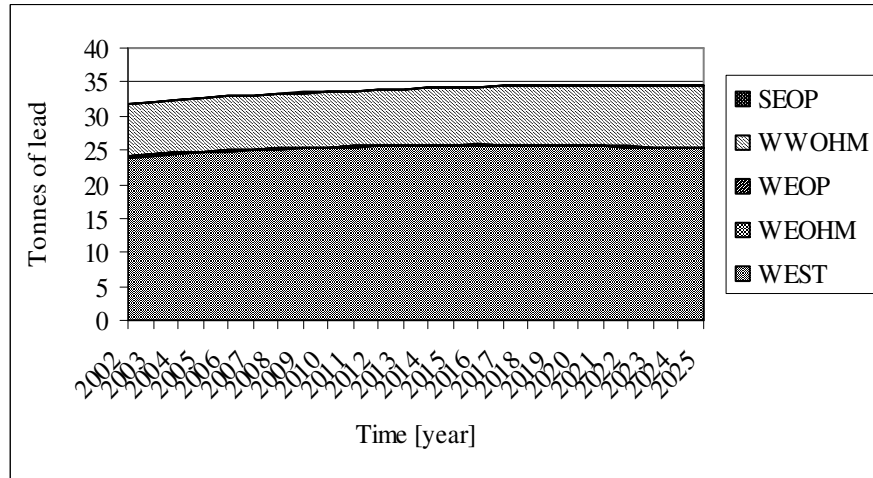
By contrast, atmospheric emissions of lead from electricity and oil production are increasing due to increase in demand for electricity and the increased production of refined oil in the NL and assumed constant emission factors for these processes.

### ***Emissions of lead to water and soil***

The factors used to estimate the water and soil emissions factors ( $\alpha_x$  in Eq. 12) are given in table 3. These provide the basis for estimating future outflows of lead to water and soil from: the production of other heavy metals (WEOHM and WWOHM) and oil refining (WEOP and SEOP respectively), and the outflow of lead to water from sewage treatment plants (WEST).



**Fig. 13:** Emissions of lead to air

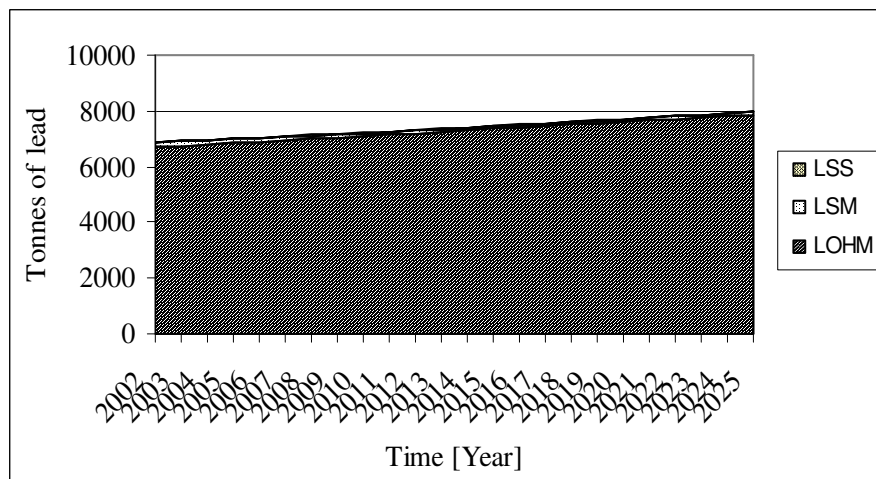


**Fig. 14:** Emissions of lead to water and soil

Figure 14 shows a slight overall increase in the total emissions of lead to water. The outflow of lead to wastewater from the production of other heavy metals is increasing due to an increase in lead input and assumed constant factor for this flow. Although, the input of lead is increasing, the emissions of lead to water from these processes are decreasing due to the assumed emission factors. The emissions of lead to water and soil from oil refining are increasing over time, due to increased activity in the NL and assumed constant emissions factors.

#### ***Lead in landfilled streams***

The factors used to estimate the lead in landfilled streams ( $\alpha_x$  in Eq. 12) are given in table 3. Based on these factors and calculations, Figure 15 shows the predicted future streams of lead in landfilled waste from several sources: the production of other heavy metals (LOHM), secondary materials (fly and bottom ashes) generated by incineration plants (LSM) and sewage sludge (LSS).



**Fig. 15:** Lead in the landfilled streams

Figure 15 shows that the outflow of lead in the landfilled stream is increasing, due to an increase in lead inputs and assumed constant factors. This figure includes the landfilled streams of secondary materials (fly ash, bottom ash and slag) generated from the production of electricity and heavy metals and incineration processes (see 4.2.1) and the landfilled stream of sewage sludge.



Leakage from landfill sites depends on many parameters, including the stock of materials (composition and amount) present at the site, the weather and hydrological conditions and the management of the site (covered or uncovered, treatment of waste water from the site etc.). The increase in lead in the landfill sites might lead to an increase in leaching of lead to the environment if these sites are not properly controlled.

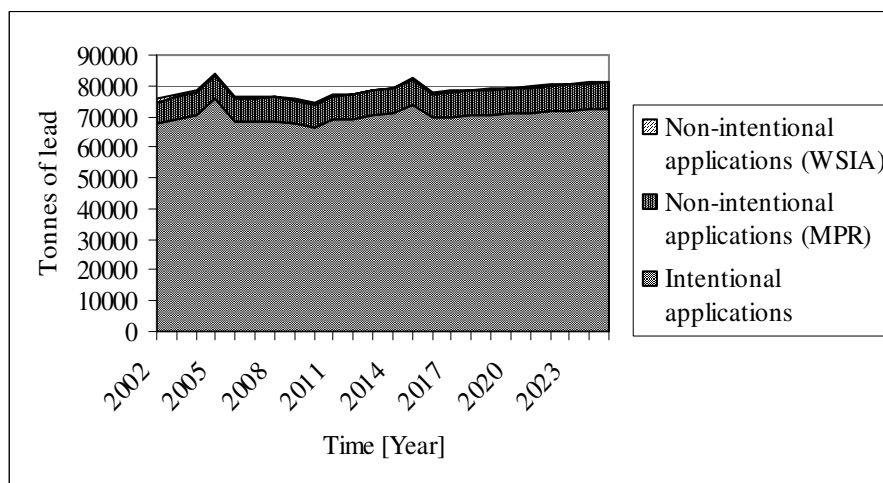
### 6.4.3 Intentional and non-intentional flows of lead

Lead enters the economy and the environment through both intentional and non-intentional flows. These inflows of lead into the economy are partly released to different environmental media and partly re-used again. The following sections compare the inflow of lead into the economy and the release of lead to the environment from its intentional and non-intentional uses.

#### *Intentional and non-intentional inflows of lead into the economy*

The intentional inflow of lead into the Dutch economy is estimated as the inflow of lead through the inflow of its main applications into the stock in use. These applications include, batteries, lead sheet in buildings, cathode ray tubes, cable sheathings, small vehicle applications, gasoline and ammunition. The non-intentional inflow of lead into the Dutch economy is estimated as the amount of lead in the coal and oil used in electricity production, in zinc and iron ores processed in the NL, in phosphate fertilizers applied to Dutch agricultural soil, in sewage sludge and in incineration residues, as discussed in 4.1.

Fig. 16 shows the inflow of lead into the economy, distinguishing between intentional use and two forms of non-intentional use, mixed primary resources (MPR) which contain lead as a contaminant and the waste streams from intentional lead applications (WSIA).



**Fig. 16:** The intentional and non-intentional inflows of lead into the economy

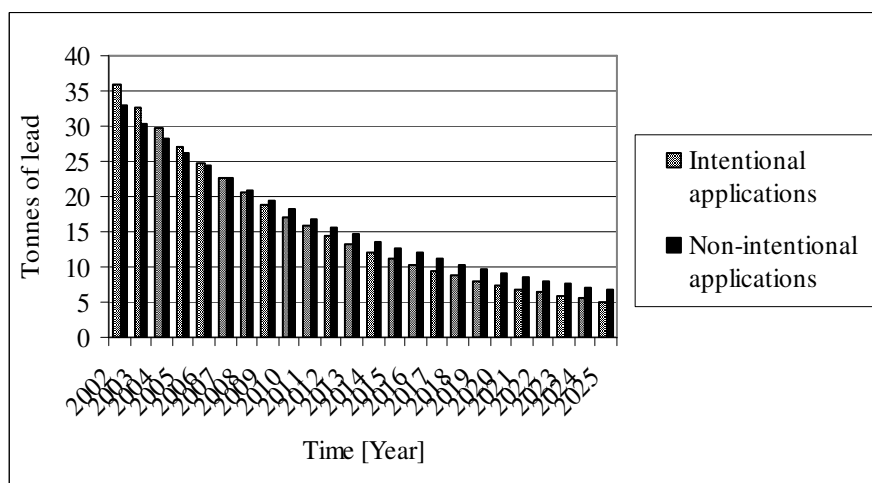
The figure shows that overall inflows of lead into the economy are slightly increasing over time. About 90% of the inflow of lead into the economy is related to intentional use. Non-intentional inflows of lead from the other two sources (MPR and WSIA) account for almost 10% of the total inflow. In 2002 about 90% of this fraction is related to the use of mixed primary resources and this is predicted to rise to 95% in 2025. The remaining 10-5 % is related to waste streams from intentional applications.

#### *Intentional and non-intentional outflows of lead to the environment*

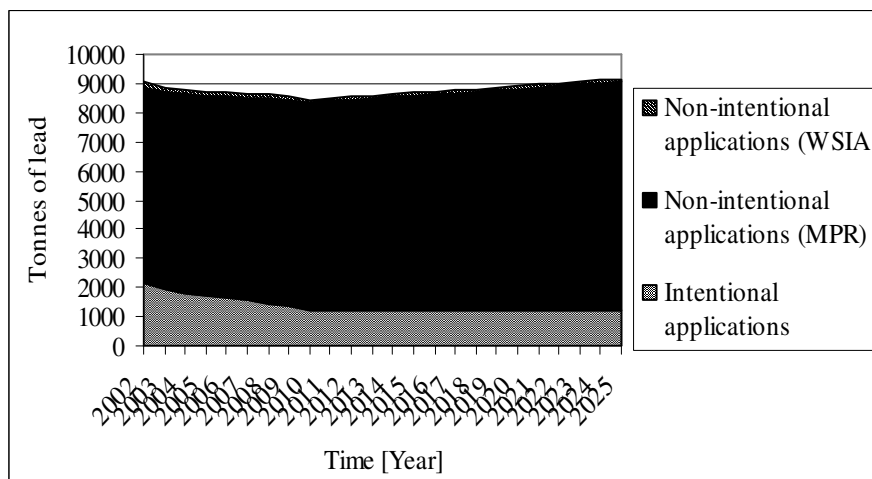
The outflows of lead to the environment from its intentional inflows are estimated as the amount of lead released to environmental compartments (air, soil and water) during the production of lead and the production, consumption, recycling and disposal of lead-containing products. The outflows of lead to the environment from non-intentional inflows are related to emissions of lead to the air, water and soil from the

production of other heavy metals (zinc, iron and steel), the production of electricity from coal and oil, the production of refined oil, the use of phosphate fertilizers, and the treatment of waste water as discussed in sections 4.2.2, to 4.2.4. Fig. 17 shows the emissions of lead to the air from both intentional and non-intentional applications. Figure 18 shows the same for landfilled streams of lead.

As shown in Fig. 17, the emissions of lead to the air from its intentional applications are greater than those related to its non-intentional applications from 2002 to 2006, but from 2006 onwards this situation is reversed. Figure 18 shows the landfilled stream of lead related to its non-intentional applications to be far greater than the stream related to the intentional applications of lead. In 2002, the landfilled stream of lead related to its non-intentional flows was 76% of the total, increasing to 87% in 2025.



**Fig. 17:** Emissions of lead to the air as a result of intentional and non-intentional applications



**Fig. 18:** Landfilled streams of lead as a result of intentional and non-intentional applications

## 6.5 Discussion and conclusions

In this chapter the non-intentional flows of lead have been modelled, their direct environmental consequences have been evaluated and a comparison made with the intentional flows of lead. The analysis was conducted using a dynamic model for the non-intentional flows of lead that combines non-intentional flows originating from waste streams from the intentional use of lead together with those originating from mixed primary resources that contain lead as a contaminant.

Regression analysis was used to determine the most variables with the greatest influence on the demand for different applications and the derived equations from the analysis were used to estimate future

developments. The expected explanatory variables, GDP, population, per capita GDP and prices, appeared to adequately explain the trends of production for electricity, oil and metals and the outcome of the regression analysis is comparable to those from other studies for the demand for these products. In the case of phosphate fertilizers, it was not possible to explain the trend of the use of fertilizers by the tested variables, due to the impact of policy. Therefore time was used as the explanatory variable since it was able to capture the influence of other time-related variables on fertilizer use.

In some cases, time is used as a proxy for technological change, policy aspects and other time-related variables. This approach is also used in the linear and exponential time models used for the analysis of the intensity of use of metals (Tiltone, 1990, Guzman et al., 1960 and Roberts, 1996). Although these models give good empirical results, they have some limitations, mainly due to the assumption that the net effect of all time related variables is constant over the time examined (Guzman et al., 1960).

The overall input of lead into the economy through a combination of direct routes (intentional flows) and indirect routes (non-intentional flows) is expected to increase in the future. The non-intentional flows of lead originating from the waste streams of intentional applications are expected to decrease over time, due to more effective recycling. However, flows of lead as a contaminant in mixed primary resources appear to be increasing. The only non-intentional inflow related to mixed primary resources that is decreasing over time is the one associated with phosphate fertilizers. This decrease is due to the policy aiming to reduce the use of chemical fertilizers in the Netherlands.

The total non-intentional outflow of lead to the air, water, soil and landfill sites is expected to increase in the future. The total emissions of lead to the air from the direct routes and indirect routes are expected to decrease in the future, while emissions of lead to water are expected to increase. In terms of pollution, the most important source of emissions of lead is the production of other heavy metals followed by sewage treatment plants. The production of iron and steel accounts for the most emissions of lead to the air, although these are decreasing due to assumptions about the emission factor. The second largest flow of lead to the air is emissions from coal-fired power plants. The incineration of the waste stream of intentional applications of lead, electricity production from oil and the production of oil make small contributions to atmospheric lead emissions.

The largest flow of lead to water originates from sewage treatment plants, followed by emissions from the production of other heavy metals and then the production of oil. All these flows are increasing over time.

The total landfilled stream of lead from the direct and indirect routes is expected to increase in the future due to the increase in the landfilled stream of lead from indirect routes. The main source of lead in landfill sites is the solid waste generated by zinc production, which is increasing over time.

The total non-intentional flow of lead in secondary materials will decrease from 2002 to 2010. This is due to the declining volumes of streams of fly ash and bottom ash generated by incineration plants, which constitute the largest flows of lead in secondary materials. The other flows of lead in secondary materials (fly ash and bottom ash from coal fired power plants, lead remains in zinc products, iron and steel slag, sewage sludge) are increasing over time.

Bottom and fly ash from incineration are the main source of available lead for possible recovery, followed by fly ash from coal fired power plants. The environmental and economic consequences of utilizing the secondary materials (fly ash, bottom ash and slag) generated from incineration plants, coal fired power plants and heavy metals production processes will be investigated in the following chapter.

Lead inputs into the economy through indirect routes (non-intentional flows) account for about 10% of the total input of lead into the economy. However these flows account for a far higher proportion of lead emissions to the environment: almost half of the emissions to air and water originate from non-intentional flows of lead, and this fraction is expected to rise in the future. Approximately three quarters of the flow of lead to landfill sites comes from non-intentional applications and this fraction is expected to increase further in the future, to 87% in 2025. Therefore in terms of both waste and emissions, the non-intentional flows are the most important ones.

The non-intentional flows of lead originating from mixed primary resource applications, especially those related to the production of zinc, iron and steel and electricity generation from coal, are larger than those originating from the waste streams of intentional applications of lead. Thus particular attention should be given to the management of the residues generated from these processes. In terms of metals, the policy aimed at increasing the incineration of sewage sludge in an attempt to minimize the amount of sludge being used on the soil or landfilled might not be effective if the incineration residues continue to be partly landfilled without the removal of the metals.

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## **Chapter 7    Long-term Consequences of Non-intentional Flows of Substances: Long Term Consequences of Substances Presence in Utilized Secondary Materials\***

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### **Abstract**

In addition to the substances' intentional or functional use, substances exist in applications as contaminants. This non-intentional presence is either due to the natural occurrence of substances in ores or due to anthropogenic sources. The presence of substances in applications as contaminants may have environmental and economic consequences.

This chapter investigates the long-term environmental and economic consequences of the existence of substances in applications as contaminants using a dynamic substance flow-stock model. The model is illustrated by non-intentional flows and stocks of lead in roads, buildings, and agricultural soil.

The model estimates the non-intentional flows of lead into different applications based on the utilized flow of the relevant materials and lead content in these materials.

The model shows that the supply of secondary material and consequently the availability of lead in non-intentional applications is increasing as the demand for electricity and other heavy metals (zinc, iron and steel) are increasing. Moreover, the reuse of road construction and building materials is leading to an increase of the availability of lead. The increase generation of secondary materials and recycling of demolished construction materials combined with possible market saturation may have environmental and economic consequences in the future. The increase availability of lead and other materials will prevent the use of secondary materials in other applications, thus increasing the stock of lead in landfill sites.

The model also shows that the monetary value of lead in the generated secondary materials is considerable. If combined with other materials that are possible to recover, the recovery of metals might be economically visible.

Key words: Substance Flow Analysis, Dynamic Modelling, Non-intentional Applications, and Lead

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## 7.1 Introduction

Large quantities of secondary materials are generated from energy and materials production related activities as a result of an increasing consumption of energy and materials and recycled demolished construction materials.

Currently secondary materials are either utilized in the construction industry or disposed in landfill sites. In the future, the market of construction material might not be able to absorb the increasing amount of secondary materials, consequently an increase in the disposal to be expected and thus an increase in the environmental and economic burden. Alternatively, a new utilization option should be found, however, the availability of substances non-intentionally in secondary materials may limit their use. On the other hand, the increase generation of secondary material can be seen as a possible solution for the expected shortage in the availability of some metals. Secondary materials contains several metals such as Lead, Zinc, Copper, Germanium, Gallium and Indium. For some metals the concentration in secondary materials is more than their concentration in their mineral resources, which make them a potential secondary sources for these metals.

This has raised the concern about the potential environmental and economic consequences of the utilization and disposal activities of secondary materials mainly due to their constitutes.

Recently, the environmental and economic consequences of the existence of substances non-intentionally in applications and the applicability of secondary materials for utilization in different areas have been the focus of several studies. The environmental and economic consequences of non-intentional flows of substances in general and the utilization of secondary materials are evaluated by the leaching test (Kosson, et al., 1996 and Nunes et al., 1996), Substance Flow Analysis (Van der Voet et al., 1994) and Life Cycle Assessment (Mroueh et al., 2001). Although, the leaching test can contribute to the study of pollution aspects related to the utilization of secondary materials, it cannot contribute to the resource aspects (Roth and Eklund, 2003). It is argued by Roth and Eklund that the leaching tests have to be complemented by the broader system boundary used in SFA and LCA to evaluate the resource and environmental impacts of the reuse of by-products in construction materials. Moreover, it is argued by Iyer and Scott, that to evaluate the applicability of secondary materials in the current utilization options and the possible new options in the future, a long-term analysis is required (Iyer and Scott, 2001).

This chapter is aimed at evaluating the long-term environmental and economic consequences of the presence of lead non-intentionally in applications using a dynamic substance flow-stock model.

SFA system represents the substance chain from cradle to grave. SFA is widely used in the study of both pollution and resources aspects. It is used to describe and analyze substance flows and stocks in the environment and the economy, identify major flows and accumulations, identify causes of pollution problems and assess the effectiveness of measures (Van der Voet, 1996). Moreover, the dynamic modelling of SFA allows for the analysis of the long-term development of the stocks and flows, the forecasts of future emissions and waste streams from built-up stocks in society and the inclusion of loops and cycles within the system (Elshkaki et al., 2004).

Lead is chosen due to its extensive use (intentionally and non-intentionally) and due to its toxic characteristics.

### Environmental consequences

Non-intentional flows find their way into the environment via several roads. Via phosphate fertilizer, lead enters the agricultural chain and accumulates there, leading to significant concentrations in manure. As a result of processing other heavy metals ores (zinc and iron ores), lead is accumulated in landfill sites, and is applied in roads materials. As a result of processing fossil fuels (coal and oil) in electricity production, lead accumulates in roads and in buildings via the use of ashes in building materials. As a result of processing lead containing waste, lead accumulates in roads, in landfill sites and in agricultural soil. The accumulated lead in roads, buildings, agricultural soil and landfill sites may leach to the soil or ground water.



## **Economic consequences**

The supply of secondary materials such as fly ash, bottom ash, slag, sewage sludge is not dependent on the demand, they are by-products of other processes. On the other hand, they are somehow inter linked within the economic system. The supply of the incineration residues (bottom and fly ashes) is ultimately linked to the demand for the intentional applications. The supply of coal-fired power plants by-products (fly and bottom ashes) and iron and steel slag is ultimately linked to the electricity demand and the demand for iron and steel. Moreover, if these materials weren't there, others would have been used which would have to be purchased. They thus replace resources. The use of fly ash in road construction materials is replacing the use of natural mineral aggregate and the use of fly ash in agriculture is replacing commercial fertilizers (Ferreira et al., 2003).

Secondary materials generated from incineration plants, coal fired power plants, production of metals, and wastewater treatment plants contain a variety of metals. These heavy metals are valuable resources that can be recovered and put to use again (Krook et al., 2004 and Tateda et al., 1997). Therefore, the remaining lead in the utilized and landfilled secondary materials without recovery can be regarded as an economic loss. On the other hand, the utilization of secondary materials in roads and buildings could reduce the economic burden associated with waste dumping. It can also reduce the use of primary resources (natural gravel and crushed rock) and the energy cost associated with their use. The presence of lead and other heavy metals in secondary materials, however, may limit their use.

## **Utilization of secondary materials**

Secondary materials generated from coal-fired power plants, incineration plants and metallurgic industry (fly ash, bottom ash and slag) are used in several applications in the area of construction industry, material recovery and agriculture. Fly ash generated from coal fired power plants, fly and bottom ash generated from the incineration of mixed solid waste and slag generated from the metallurgic industry are utilized mainly in road and building construction materials, however, these secondary materials can also be utilized in several other applications. Coal fired power plants fly ash can be utilized in the production of zeolites which is suitable for application as an immobilizer for air pollutants, the production of Glass materials and composite materials, adsorbent for waste management, waste stabilization, and materials recovery (Iyer and Scott, 2001). Coal-fired power plants fly ash can also be used in land applications with and without sewage sludge (Sajwan et al., 2003). Fly ash generated from the incineration of mixed solid waste can be utilized in agriculture either as fertilizer or amendment, in the production of adsorbing materials, and as sludge conditioning (Ferreira et al., 2003).

## **Recovery of metals**

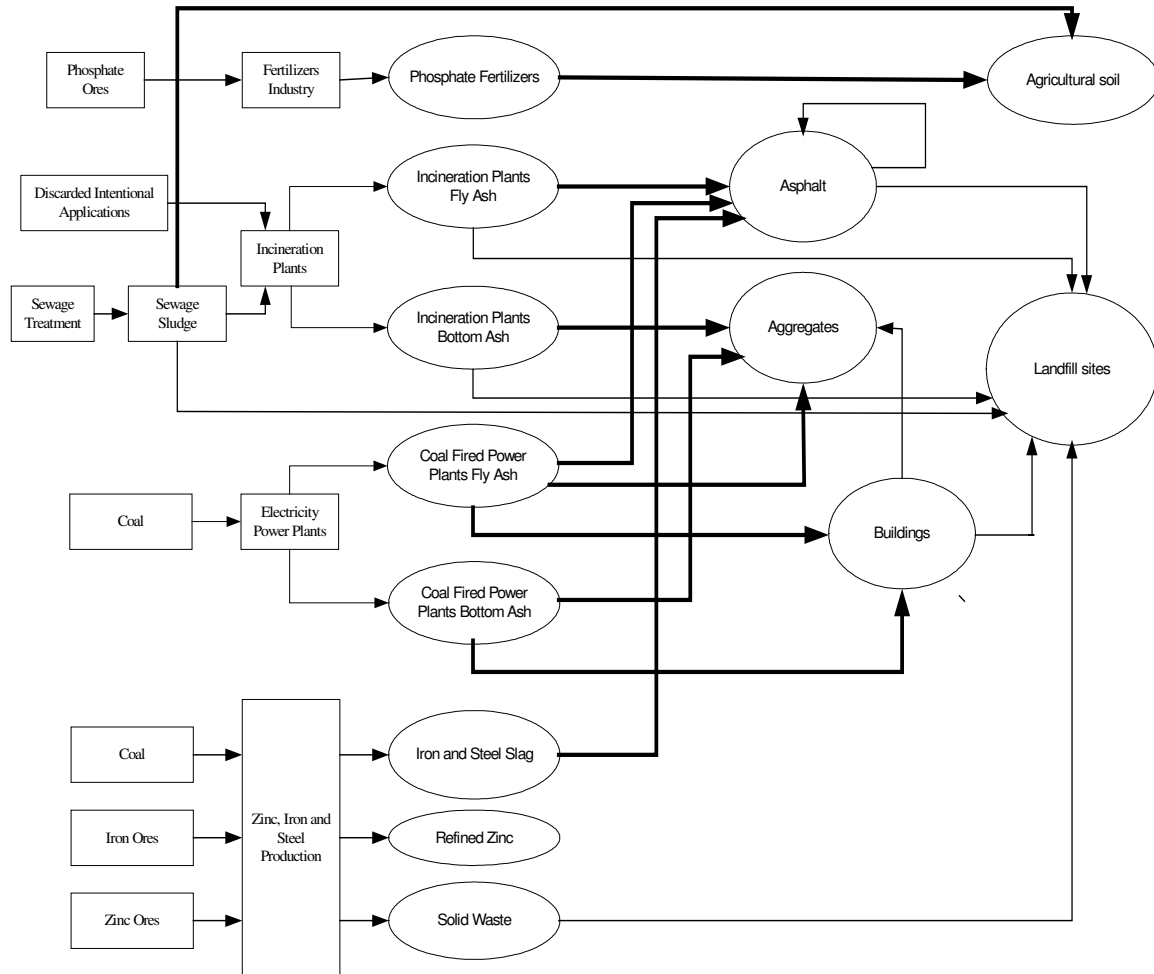
Several studies are conducted to examine the recovery of metals from fly ash generated from the incineration plants (Nagib and Inoue, 2000 and Izumikawa, 1996). Nagib and Inoue reported the possibility of recovering more than 97% of lead and 68% of zinc from fly ash generated from municipal incineration plants by acid and/or alkaline leaching and Izumikawa reported the possibility of recovering almost 100% of the heavy metals (Izumikawa, 1996).

Metals such as Iron, gallium, vanadium, nickel and magnesium can also be recovered from coal fly ash (Fang and Gesser, 1996 and Murase et al. 1998).

Tateda et. al estimated the losses of lead from municipal solid waste incineration ash, thermal power station coal ash, and sludge incineration ash from wastewater treatment facilities in Japan to be 22162 ton of lead/year and the monetary losses of 10.4 million dollar/year (Tateda et al., 1997).

## 7.2 Methodology

The non-intentional flows and stocks of lead originate from coal fired power plants, production of heavy oil, iron and steel, zinc and copper, waste water treatment, and the incineration of lead intentional applications are shown in figure 1.



**Fig. 1:** Lead non-intentional flows and stocks in the Dutch economy and environment

### 7.2.1 General setup of the model

### *Modelling lead inflow into the stock of non-intentional applications*

The inflow of lead into the stock of a certain non-intentional application (road construction materials) or landfill sites from a specific secondary materials (fly ash, bottom ash) is estimated based on the amount of lead in the generated stream of secondary material and the utilized fraction of this stream as given by Eq. 1.

$$F_{L,x,app}^{in}(t) = \beta_x(t) \cdot F_{L,x}^{out}(t) \quad (1)$$

$F_{L,x,app}^{in}(t)$  is the inflow of lead from a certain secondary material into the application at time  $t$ ,  $F_{L,x}^{out}(t)$  is the outflow of lead in the generated secondary material from a certain process at time  $t$  and  $\beta_x$  is the utilization factor at time  $t$ .

The inflow of lead through a specific secondary material into landfill sites is estimated as given by Eq. 2.

$$F_{L,x,L}^{in}(t) = F_{L,x}^{out}(t) - F_{L,x,app}^{in}(t) \quad (2)$$

$F_{L,x,L}^{in}(t)$  is the inflow of lead from a certain secondary material into the landfill sites at time t

### ***Modelling lead outflow from the stock of non-intentional application***

The outflow of lead out of the stock of road construction materials takes place through two processes: leaching and delay. Leaching may occur during use and delay is related to the discarding of products after use.

The discarded outflow of a certain product depends mainly on the product inflow and its life span. The discarded outflow is estimated as a delayed inflow, corrected for the leaching that have taken place during use, as given by Eq. 3:

$$F_D^{out}(t) = F_C^{in}(t - L_U) - \sum_{i=1}^{L_U} C \cdot F_C^{in}(t - L_U) \cdot (1 - C)^{i-1} \quad (3)$$

Where  $F_D^{out}(t)$  is the outflow due to the delay mechanism at time t and  $L_U$  being the life span of the product in use.

The leaching outflow is estimated as a fraction of lead stock as given by Eq. 4.

$$F_E^{out}(t) = C \cdot S(t) \quad (4)$$

Where  $F_E^{out}(t)$  is the leaching outflow at time t, C being the emission factor and S is the stock

### ***Modelling lead accumulation in non-intentional application***

The change of the magnitude of the stock over time is the difference between the inflow and the outflow as given by Eq. 5.

$$\frac{dS}{dt} = F^{in}(t) - F^{out}(t) \quad (5)$$

$F^{in}(t)$  is the inflow of lead through the utilized streams at time (t),  $F^{out}(t)$  is the outflow of lead at time (t).

## **7.2.2 Estimation of lead inflows into stock-in-use of non-intentional applications**

### ***Road construction materials (aggregates and asphalt)***

#### ***Road construction materials (Aggregate)***

The inflow of lead into the stock of road aggregates originates from two sources: bottom ash generated from the incineration of lead intentional applications and sewage sludge (BAIN) and bottom ash and fly ash generated from coal fired power plants (BAC and FAC).

$$F_{agg}^{in}(t) = F_{UBAIN}^{in}(t) + F_{UBAC}^{in}(t) + F_{UFAC}^{in}(t) \quad (6)$$

The past inflow of lead into the stock of road construction materials (aggregates) through the utilized stream of bottom ash generated from the incineration plants (UBAIN) from 1980 through 2001 is estimated based on the incinerated mixed solid waste stream and the quantity of BAIN being applied in road construction materials (aggregates), combined with data on the lead content of this stream. Data on the

utilized stream of BAIN from 1988 through 2001 are available (VVAV, 2001). Before 1988, no data are available. We assume that the use started in 1980, and that the utilized amount of BAIN in the Netherlands before 1988 is the same as the amount in 1988. The lead content in BAIN is assumed to be 1500 mg lead/kg ash (Kosson, et al., 1996).

The future inflow of lead into the stock of road construction materials (aggregates) from BAIN is estimated as given by Eq. 1. The partitioning of lead to BAIN and the utilization factor, which are estimated based on (Sloot, 1996), are given in table 1. The utilization factor of BAIN in the past is assumed to be valid for the future.

**Table 1:** The amount of lead in the generated secondary materials and their utilization fractions

Flow	Partitioning of lead	Utilization factors
BAIN	68%	90% as aggregate
FAIN	32%	50% as asphalt
BAC	4%	47% as aggregate 53% as building materials
FAC	95.6%	20% as aggregate 20% as asphalt 60% as building materials
SPIS	12.1%	100% as asphalt
SS	80%	15% for land preparation

The past and future inflow of lead (from 1987 onwards) into the stock of road construction materials (aggregates) through the utilized stream of bottom ash generated from coal fired power plants (UBAC) is estimated as given by Eq. 1. The partitioning of lead to BAC (Sandelin and Backman, 2001 and Sandelin et al. 1999), and the utilization factor (VVAV, 2001), are given in table 1. From 1980 through 1987, the inflow of lead is assumed to be the same as the inflow in 1987.

The past and future inflow of lead (from 1987 onwards) into the stock of road construction materials (aggregates) through the utilized stream of fly ash generated from coal-fired power plants (UFAC) is estimated as given by Eq. 1. The partitioning of lead to FAC (Sandelin and Backman, 2001 and Sandelin et al. 1999), and the utilization factor of FAC (Eymael and Cornelissen, 1996), are given in table 1. From 1980 through 1987, the inflow of lead is assumed to be the same as the inflow in 1987.

### **Road construction materials (Asphalt)**

The inflow of lead into the stock of road construction materials (asphalt) originates from three sources: fly ash generated from the incineration of lead non-intentional applications and sewage sludge (FAIN), fly ash generated from coal fired power plants (FAC) and iron and steel slag (SPIS). Recycling might further influence the stocks. When old asphalt is reused to produce new, a closed loop might evolve leading to ever increasing concentrations of lead.

$$F_{asph}^{in}(t) = F_{UFAIN}^{in}(t) + F_{UFAC}^{in}(t) + F_{USPIS}^{in}(t) + F_{UR}^{in}(t) \quad (7)$$

The past inflow of lead into the stock of road construction materials (asphalt) through the utilized stream of fly ash generated from the incineration plants (UFAIN) from 1980 through 2001 is estimated based on the incinerated mixed solid waste stream and the quantity of FAIN being applied in road construction materials (asphalt), combined with data on the lead content of this stream. Data on the utilized stream of FAIN from 1988 through 2001 are available (VVAV, 2001). Before 1988, no data is available. We assume that the use started in 1980, and that the utilized amount of FAIN in the Netherlands before 1988 is the same as the amount in 1988. The lead content in FAIN is assumed to be 4000 mg lead/kg, based on (Kosson, et al., 1996).

The future inflow of lead into the stock of road construction materials (asphalt) from FAIN is estimated as given by Eq. 1. The partitioning of lead to FAIN (Sloot, 1996) and the utilization factor (Sakai et al., 1996) are given in table 1. The utilization factor of FAIN in the past is assumed to be valid for the future.

The past and future inflow of lead (from 1987 onwards) into the stock of road construction materials (asphalt) through the utilized stream of fly ash generated from coal fired power plants (UFAC) is estimated as given by Eq. 1. The partitioning of lead to FAC and the utilization factor of FAC are given in table 1. From 1980 through 1987, the inflow of lead is assumed to be the same as the inflow in 1987.

The past and future inflow of lead into the stock of road construction materials (asphalt) through the utilized stream of the slag generated from iron and steel production (USPIS) from 1980 onwards is estimated as a fraction of lead input through iron ores and coal used in steel production.

The inflow of lead through iron ores is estimated as 0.2 kg of lead per ton of iron and the inflow of lead through coal is estimated as 8.32E-3 kg of lead per ton of steel.

### ***Building materials***

The inflow of lead into the stock of buildings materials originates from bottom ash (BAC) and fly ash (FAC) generated from coal fired power plants.

$$F_{build}^{in}(t) = F_{UFAC}^{in}(t) + F_{UBAC}^{in}(t) \quad (8)$$

The past and future inflow of lead (from 1987 onwards) into the stock of building materials through UBAC is estimated as given by Eq. 1. The partitioning of lead to BAC and the utilization factor of BAC are given in table 1. From 1980 through 1987, the inflow of lead is assumed to be the same as the inflow in 1987.

The past and future inflow of lead (from 1987 onwards) into the stock of building materials from through UFAC is estimated as given by Eq. 1. The partitioning of lead to FAC and the utilization factor FAC are given in table 1. From 1980 through 1987, the inflow of lead is assumed to be the same as the inflow in 1987.

### ***Materials used in agricultural soil***

The inflows of lead into the agricultural soil originate from four sources: air, phosphate fertilizers, sewage sludge, and manure.

$$F_{agrsol}^{in}(t) = F_{ag,air}^{in}(t) + F_{ag,fert}^{in}(t) + F_{ag,SS}^{in}(t) + F_{ag,manure}^{in}(t) \quad (9)$$

The past and future non-intentional flow of lead through phosphate fertilizers is estimated on the basis of the past and future use of phosphate fertilizers and the amount of lead in fertilizers. The amount of lead in fertilizers is estimated as 0.135 kg of lead per ton of fertilizer (Annema et al., 1995).

Lead in sewage sludge is partly ends up in agricultural soil due to the use of sewage sludge in land preparation. The inflow of lead into the agricultural soil through sewage sludge is estimated as 15% of the total lead in sewage sludge. Lead in sewage sludge is estimated as 80% of total lead input to sewage treatment plants.

The inflow of lead as a result of using manure is treated as internal loop in the agricultural sector.

### 7.2.3 Estimation of non-intentional outflows of lead from stock-in-use

#### *Road construction materials (aggregates and asphalt)*

The outflow of lead out of the stock of road construction materials takes place through two processes: leaching and delay.

Leaching may occur during use of road construction materials as a result of processes in the soil, which may free the lead out of the road materials. The release of lead from road construction materials is determined by the availability of lead, fill depth, infiltration rate, lead solubility as a function of residue PH (Kosson, et al., 1996). Kosson et al. evaluated the cumulative release of lead over 100 years for several management options (road construction materials and disposal). They report a release of small amount of lead, below the maximum level of increasing the soil concentration over 100 years (85mg Pb/kg). Using liner system and leachate collection reduces the actual environmental impact of the disposal or utilization. Although there is a release of small amount of lead from road construction materials, the leaching flow will be ignored due to the conclusions of several studies that this flow does not have environmental consequences and due to the fact that the flow is too small to effect the discarded outflow.

Delay is related to the discarding of products after use. The discarded outflow of a certain product depends mainly on the product inflow and its life span. The discarded outflow is estimated as a delayed inflow, corrected for the leaching that have taken place during use, as given by Eq. 3:

For road aggregates, we assume that the aggregate is not being replaced but stays in place as long as the road is there. That implies that the stock of lead in aggregates is treated as a sink: no outflow takes place at all. Road asphalt is replaced frequently in the process of maintenance and repair of the roads. The average life span of asphalt on the Dutch roads is unknown. We assume, arbitrarily, an average life span of 10 years. Therefore, the only outflow accounted for in road construction materials is the outflow of lead in asphalt due to the delay mechanism as given by Eq. 3. The discarded outflow of asphalt is reused in road construction materials with almost 100% (Schimmoller, 2000).

#### *Buildings materials*

The outflow of lead out of the stock of building materials takes place through two processes: leaching and delay. The yearly emissions of lead from buildings material is ignored due to the same reasons mentioned for road construction materials (Ferreira et al., 2003). The discarded outflow is estimated as given by Eq. 3. The average life span of building materials is assumed to be 50 years.

The discarded outflow of building materials is reused in road construction materials with almost 100% (Schimmoller, 2000).

#### *Materials used in agricultural soil*

The outflows of lead from the agricultural soil take place through the uptake of lead by food and fodder and the leaching to the ground water. The three outflows are estimated as a fraction of the lead stock in agricultural soil as given by Eq. 4. The uptake coefficients for food and fodder are estimated as 0.0018 and 0.0142 respectively. The leaching rate is estimated as 0.0182.

### 7.2.4 Estimation stocks of lead in the economy

The change of the magnitude of the stock over time is the difference between the inflow and the outflow as given by Eq. 5.

#### *Road construction materials (aggregates and asphalt)*

The stock of lead in road construction materials (aggregates) from 2003 onwards is estimated as given by Eq. 5. The initial stock of lead in aggregates in 2002 is estimated based on the utilized stream from 1980 through 2001 of BAIN, BAC and FAC as given by Eq. 10.

$$ISAG(t) = \sum_{t=1980}^{2001} F_{UBAIN}^{in}(t) + F_{UBAC}^{in}(t) + F_{UFAC}^{in}(t) \quad (10)$$

The stock of lead in road construction materials (asphalt) from 1991 onwards is estimated as given by Eq. 5. The initial stock of lead in asphalt in 1990 is estimated based on the utilized stream from 1980 through 1990 of FAIN, FAC, and SPIS as given by Eq. 11.

$$ISAS(t) = \sum_{t=1980}^{1990} F_{UFAIN}^{in}(t) + F_{UFAC}^{in}(t) + F_{USPIS}^{in}(t) \quad (11)$$

The stock is further influenced by recycling. The discarded asphalt is reused with almost 100% in the Netherlands [24].

### ***Buildings materials***

The stock of lead in building materials from 1991 onwards is estimated as given by Eq. 5. The initial stock of lead in buildings in 1990 is estimated based on the utilized stream from 1980 through 1990 of FAC and BAC as given by Eq. 12.

$$ISB(t) = \sum_{t=1980}^{1990} F_{UFAC}^{in}(t) + F_{UBAC}^{in}(t) \quad (12)$$

### ***Materials used in agricultural soil***

The stock of lead in agricultural soil from 2002 onwards is estimated as given by Eq. 5. The initial stock of lead in agricultural soil in 2001 is estimated based on the accumulated amount of lead from 1980 through 2000 (CBS, 2003).

## **7.2.5 Estimation of the economic consequences**

The economic consequences of the presence of lead and other metals in secondary materials are not limited to the value of these metals but also to the economic benefit due to the saving in the costs associated with materials dumping and the use of primary materials. The analysis presented here is limited to the economic value of the recovered lead from secondary materials, however, to estimate the economic benefit of metals recovery, the value of the other metals exist in secondary materials, which could have a higher value than lead such as indium, germanium, and gallium, and the cost of their recovery should be included. Several authors proposed extraction processes of metals from secondary materials which believed to be economically feasible and the cost of the end products compete with market price for the same primary compounds (Fang and Gesser, 1996, Basir and Rabah, 1999 and Nagib and Inoue, 2000).

### **The value of the metals in the utilized flows of secondary materials**

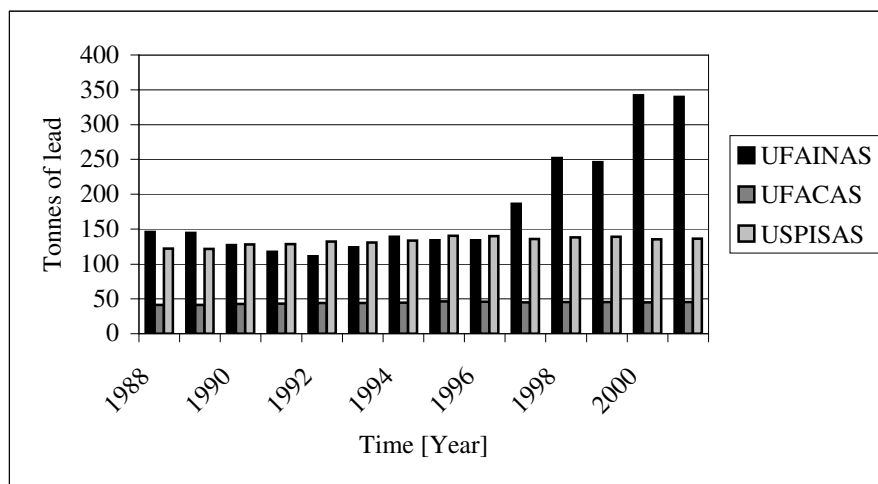
The amount of lead in the utilized flows of secondary materials (UFAIN, UBAIN, USS, USPIS, UFAC and UBAC) is estimated as described in section (2.2). The economic losses due to the remaining lead in the utilized secondary materials are estimated on the basis of the amount of lead in these streams multiplied by lead price as given by Eq. 13.

$$\text{The monetary losses} = \text{lead price} * (\text{UFAIN} + \text{ULBAIN} + \text{USS} + \text{USPIS} + \text{UFAC} + \text{UBAC}) \quad (13)$$

## 7.3 Model results

### 7.3.1 Non-intentional inflows of lead into stock-in-use

Past inflows of lead into road construction materials (asphalt) through the utilized stream of the incineration fly ash (UFAIN), coal fired power plants fly ash (UFAC), iron and steel slag (USPIS) are shown in figure 2 and the future inflows of lead from FAIN, FAC, SPIS and the recycled asphalt (RAS) are shown in figure 3. The main flow of lead into road construction materials (asphalt) originates from the recycled asphalt, which is increasing due to the past development in the utilized streams in asphalt. The second largest flow originates from SPIS, which is increasing as a result of increasing demand for iron and steel. The third flow originates from FAIN, which is decreasing from 2002 through 2010 and stabilizing from 2002 onwards as a result of lead input into the incineration plants. Small contribution to lead in asphalt from FAC, which is slightly increasing as a result of increasing demand for electricity.



**Fig. 2:** Lead inflows into the stock of road construction materials (asphalt)

Future inflows of lead into road construction materials (aggregates) through the utilized stream of the incineration bottom ash (UBAIN) and coal fired power plants fly and bottom ashes (UBAC and UFAC) are shown in figure 3. The main flow of lead into road construction materials (aggregates) originates from BAIN. The inflow is decreasing from 2002 through 2010 and stabilizing from 2010 onwards. This is ultimately a result of the input of lead into the incineration plants. Although the input of lead into the incineration plants from the sewage sludge is increasing, the input from the discarded intentional applications is decreasing as a result of increasing recycling. The second largest flow of lead originates from FAC, which is increasing as a result of increasing demand for electricity. A small contribution to lead in aggregates from BAC.

Future inflows of lead into building materials from coal fired power plants fly ash (FAC) and bottom ash (BAC) are shown in figure 3. The main flow of lead into building materials originates from FAC followed by BAC. Both are increasing as a result of increasing demand for electricity.

The total future inflows of lead into the stock of road construction materials and building materials from different sources are shown in figure 3. The model shows that the inflow of lead into the stock of road construction and building materials vary by secondary materials sources.

Lead inflows into the agricultural soil from air, fertilizers, sewage sludge, and manure are shown in figure 4. The main flow of lead into agricultural soil originates from manure, which is increasing as a consequence of both the intentional and non-intentional applications.

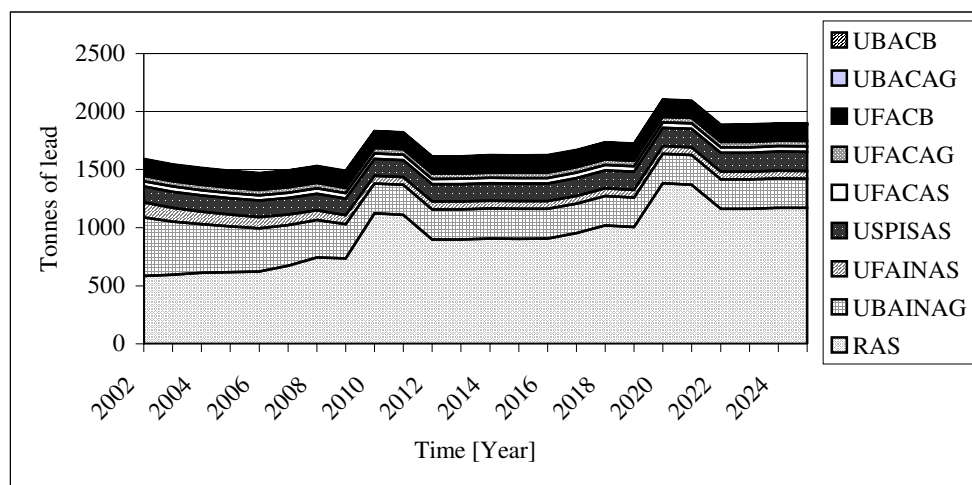


Although, the inflow of lead originates from phosphate fertilizers is decreasing due to the policy in the NL, the inflows of lead from sewage sludge and manure are increasing.

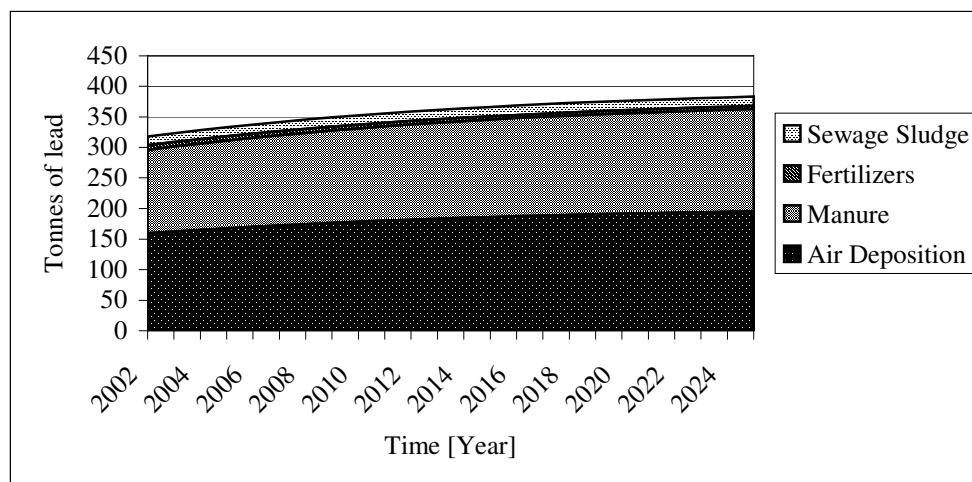
The landfilled stream of incineration residues (bottom and fly ashes) is decreasing from 2002 through 2010 and then stabilizing. This is due to the input of lead into the incineration plants.

The landfilled stream of sewage sludge is increasing from 2002 through 2016 and from 2017 onwards slightly decreasing. This is mainly due to the development in the sources of lead in sewage treatment plants, the production of other heavy metals, consumption of animal and food products, and the emissions from the use of lead intentional applications.

The landfilled flow of solid waste generated from the production of other heavy metals is increasing due to an increase demand for other heavy metals.



**Fig. 3:** Lead inflows into road construction and building materials



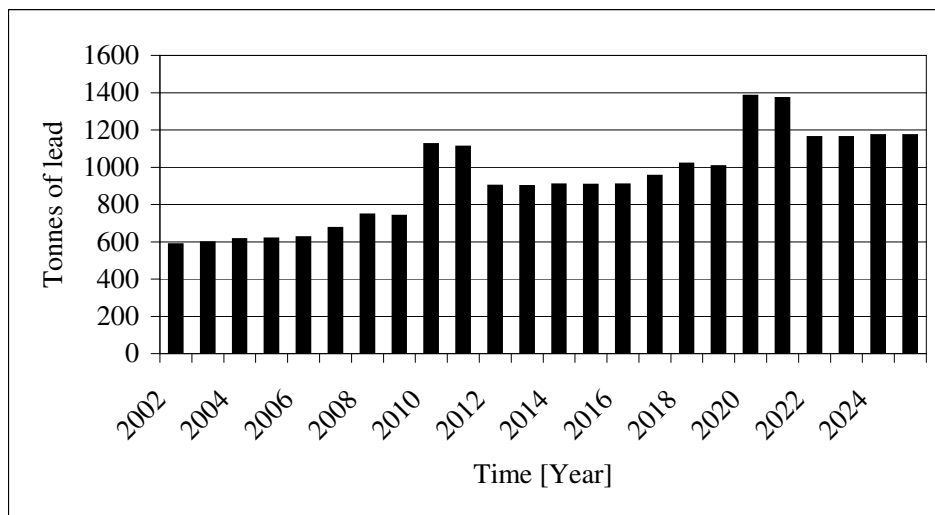
**Fig. 4:** Lead inflows into agricultural soil

### 7.3.2 Non-intentional lead outflows from stock-in-use

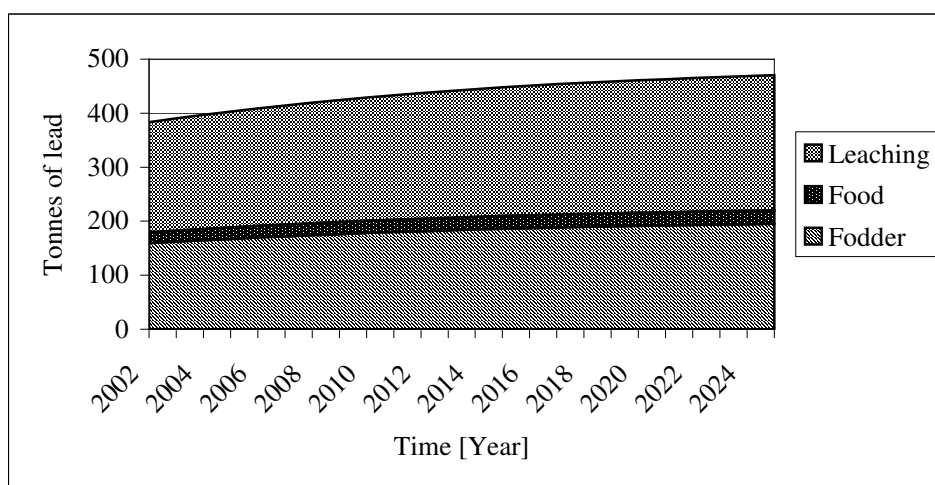
The only outflow of lead from road construction and building materials in the studied time is the discarded outflow of asphalt, the discarded outflow of building materials will start to come out of buildings in 2030.

Lead discarded outflow from road construction materials (asphalt) is shown in figure 5. The outflow is increasing overtime due to the past development in the utilized streams in asphalt.

Lead uptakes by food and fodder from agricultural soil and the leaching flow are shown in figure 6. The outflows from agricultural soil are the uptakes by food and fodder. Both are increasing as a result of the increasing stock of lead in agricultural soil.



**Fig. 5:** Lead discarded outflow from the stock of road construction materials (asphalt)



**Fig. 6:** Lead outflows from the agricultural soil

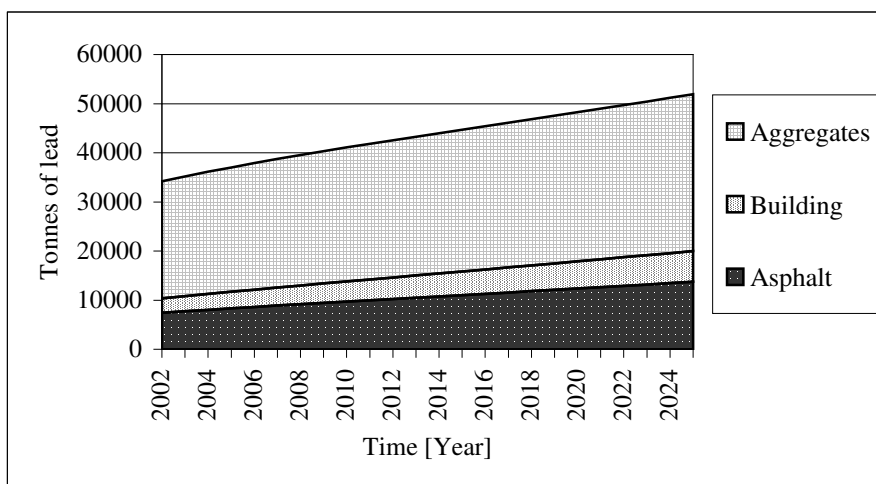
### 7.3.3 Stocks of lead in the economy

Stocks of lead in road construction materials (aggregates and asphalt) and building materials are shown in figure 7 and the stock of lead in agricultural soil is shown in figure 8.

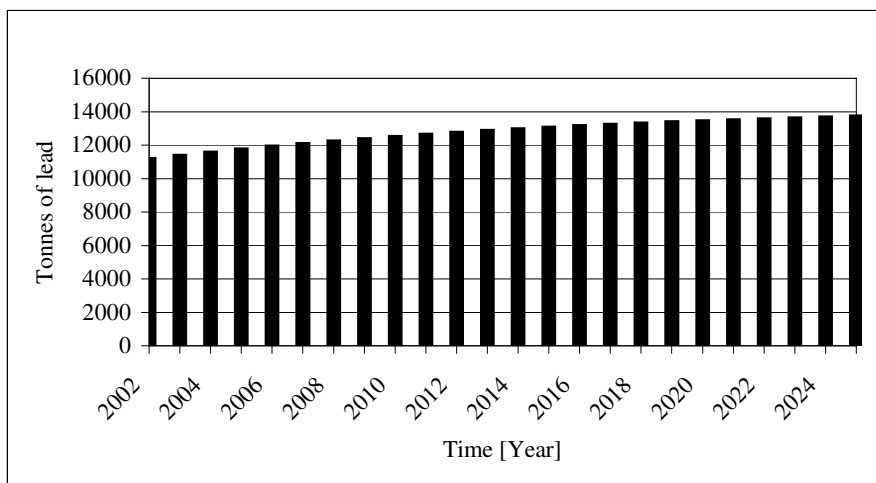
Stocks of lead in road construction and building materials are increasing due to the long life span of some of these materials and the high level of recycling. Lead stock in agricultural soil is increasing. The increase in the stock of lead in agricultural soil is partly related to the intentional applications of lead.

### 7.3.4 Long-term economic consequences of non-intentional lead flows

The largest stream containing lead and therefore the largest economic value, is the one generated from the incineration plants. The second largest stream is the generated secondary materials from coal fired power plants. Although, the monetary value of lead in the utilized streams of SS, SPIS, FAC and BAC is increasing overtime due to the increase generation of these materials, the overall monetary value of lead is decreasing from 2002 through 2010 and increasing slightly afterwards. This is mainly due to the development in the incineration of lead intentional applications.



**Fig. 7:** Lead stocks in road construction and building materials



**Fig. 8:** lead stocks in agricultural soil

## 7.4 Discussion and conclusions

The model presented in this chapter is a dynamic substance flow-stock model of lead non-intentional applications.

The inflows of lead into the stock of road construction materials and building materials are mainly determined by the generation of secondary materials and the utilized stream of these materials. The generation of secondary materials is determined by the demand for lead intentional applications, electricity, petroleum products and other heavy metals. The utilization of secondary materials is mainly determined by technical, environmental and economic factors.

The outflows of lead from the stock of road and building construction materials are those related to the discarded asphalt and building materials. The leaching flows is ignored due to the conclusions by several studies that these flows are too small and below the toxicity level and due to the fact that these flows are too small compared to the discarded outflows.

The stocks of lead in road and building construction materials are increasing due to the increase utilization of secondary materials and the reuse of the discarded materials. The increase of lead in the stock might limit the future utilization of secondary materials and the recycalability of the discarded materials.

The main source of lead in the utilized streams of secondary materials is the generated fly and bottom ashes from the incineration plants followed by those generated from coal fired power plants.

The main source of lead in landfill sites is the solid waste stream generated from the production of zinc followed by the landfilled streams of fly ash and bottom ash generated from the incineration.

The inflows of lead from secondary materials generated from coal fired power plants and the production of other heavy metals are increasing overtime and those generated from the incineration plants are decreasing from 2002 through 2010. The increase in secondary materials generated from coal fired power plants and the production of other heavy metals is mainly due to the increase demand for electricity, zinc, iron and steel and the decrease of those generated from the incineration plants is due to the waste management policy, which is leading to an increase in the recycling of lead intentional applications.

At present, the generated streams of secondary materials BAIN, FAIN, BAC, FAC, and SPIS are utilized with almost 90%, 50%, 100%, 100%, 100% respectively in road and building construction materials due to their technical and environmental acceptance. This is might not be the case in the future.

The generation of secondary material and the recycling of discarded construction materials are increasing overtime. If this combined with a possible market saturation for construction material, the amount of secondary materials to be landfilled is going to increase. Otherwise, alternative utilization options for secondary materials should be found, however, the presence of lead and other heavy materials might limit the possibility of utilizing secondary materials in other areas.

The recovery of substances from secondary materials will allow for the utilization of secondary materials in other areas, consequently minimizing the environmental and economic burden associated with landfilling.

The monetary value of lead in the utilized streams is considerable, if combined with other heavy metals in mixed solid waste, coal, oil and other metals ores, which also can be recovered from secondary materials (Fang and Gesser, 1996, Murase et al, 1998, Nagib and Inoue, 2000 and Izumikawa, 1996), the recovery of these metals might be economically visible. Moreover, the losses of lead in landfilled streams are 7 times more than the losses of lead in the utilized streams.

The economic analysis is limited to the value of lead in secondary materials, however, a more detailed cost benefit analysis is needed in which the value of all materials that can be recovered and the costs of their recovery, in addition to the other benefits in terms of reducing the demand for the land required for landfill and primary materials are included.

The analysis present in this chapter is made for lead flows and stocks in the NL, however, the generation of secondary materials in the NL from coal for example is small compared to other countries, which rely more on coal for their electricity production. From resource prospective, the analysis should be extended for other metals and other countries.

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## Chapter 8    The Consequences of the Use of Platinum in New Technologies on its Availability and on Other Metals Cycles \*

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### Abstract

Recently, fuel cell vehicles (FCV) are being developed to reduce the environmental impacts related to the conventional internal combustion engine vehicles. Although on the short term the newly proposed technology might serve the intended purpose. On the long term, there may be bottlenecks in the supply of specific metals required for the technology and new emissions may replace the old ones.

Fuel cell technology requires the use of platinum, which is cited as a possible bottleneck for a more widespread use of the new technologies. Moreover, an increase in platinum demand ultimately implies an increased production of the co-produced metals Cu and Ni. Consequently an increased supply may well have environmental consequences on Ni and Cu recycling system.

The chapter is aimed at

- Investigating the potential long-term impact of the increase use of platinum in fuel cell technology and other applications in terms of resource depletion
- Evaluating the long-term consequences of the increased demand of platinum on the cycles of other co-produced metals especially Ni and Cu

The analysis is carried out using a dynamic substance flow-stock model for platinum, nickel and copper.

The model consists of a set of differential equation describing the change of the magnitude of the substance stock in the system compartments (production, use and waste management of platinum applications, primary production of platinum in South Africa, Russia, USA, Canada and others and secondary production of platinum) over time and several model relations. The model is implemented in Matlab/SIMULINK environment.

The main driving force in the model is the global demand for platinum. The global demand for platinum is estimated based on the demand for its applications (fuel cell, catalytic converters, and the other applications) and platinum required for each application. In turn, the demand for platinum applications are modelled based on socio-economic variables such GDP, per capita GDP, population size, material price and the cost of these applications. Platinum required for each application is modelled as a function of cumulated production using the learning curve. In addition, several other factors are important in determining the main outcome such as the applications life span, the applications collection rates and the efficiency of the production processes (primary and secondary).

The main model outcomes are the amount of primary platinum required for FCVs and other applications and the consequences on platinum current reserve, platinum identified resources and the co-produced metals recycling and primary production from other ores.

The model shows that the demand for primary platinum will increase dramatically with the introduction of FCVs despite the possibility of the decrease of platinum loading of FC. This is mainly due to the increased demand for vehicles. Without changes in management, the current platinum reserve would be exhausted in three decades and the identified resources in roughly 60 years. The model also shows that the demand for the co-produced materials is increasing over time. The supply of these metals from Pt ores is, combined with only a part of their current secondary production, sufficient to meet the rising demand. Consequently the primary production of these metals from other ores than those of Pt ores will not be needed. Recycling of these metals is expected to decrease.

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\* Reprinted from “Elshkaki, A., Van der Voet, E. (2006). Conservation and Recycling of Resources: New Research”.

## 8.1 Introduction

The increase in global population and the growth in consumption per head have led to an increase in materials and energy use. This has raised the concern about the exhaustion of limited resources and the environmental impact of resources during their life cycle.

Several new technologies for sustainable development in the field of energy production, nanotechnologies and ICT aim at reducing the environmental pressure by decreasing the use of (fossil) energy and materials. Some of these technologies require the use of specific metals. Among these are platinum and palladium that are required for car catalysts and fuel cells technologies, indium and germanium that are required for solar cell technologies, and bismuth and germanium, in the case of lead free electronic solder.

On the short term, each of the proposed technologies may serve the intended purpose of reducing environmental impact. Combined and on the long term, however, there may be bottlenecks in the supply of the required metals and new emissions may replace the old ones. The proposed technologies might reduce the environmental impacts related to the use of resources, however, on the long term, firms might start extracting low-grade ores to meet the demand for the required materials. This will lead to the use of more energy and will produce more waste. Another concern stems from the fact that platinum and palladium are mostly co-produced with other, more abundant metals such as copper and nickel. The link between the required metals and their "host" metals in nature may have negative impacts on the host metals cycles. An increase in the demand for Pt or Pd ultimately implies an increased production of these host metals. This may well have environmental consequences, the more so as lower prices will make extraction of the metals from wastes for recycling less attractive.

The assessment of the new technologies requires the inclusion of all above-mentioned environmental impacts in terms of long term availability of resources, emissions and waste generation, energy use, and co-produced metals.

This chapter treats a case in point to illustrate the importance of the abovementioned problems. The long term potential use of platinum in fuel cells is evaluated in terms of platinum resource availability and the co-produced metals supply and demand. The other aspects are mentioned briefly.

Platinum is a rare metal with a concentration of 5 part per billion (ppb) (British Geological Survey, 2005) in the earth crust. Platinum can be found in nature in three different types of ores; PGE dominants ores, Ni-Cu dominant ores and miscellaneous ores (Xiao and Laplante, 2004). Recently fuel cell vehicles are being developed to reduce the environmental impacts related to the conventional internal combustion engine vehicles. Fuel cell technology, one of the main items required for these vehicles, requires the use of platinum as an important element of the electrodes of the proton exchange membrane fuel cell (PEMFC). Pt is used to promote the rate of the electrochemical reactions required for  $H_2$  to release electrons and become  $H_2$  ions. In addition to the new proposed technologies, platinum is currently used in several applications due to its chemical and physical properties. It is used in catalytic converters to reduce the emissions of hydrocarbons, carbon monoxide, nitrogen oxide, and other atmospheric pollutants from vehicle exhausts. It is widely used in industrial applications (chemical, petrochemical, glass, and electrical and electronics) due to its relative inertness and its ability to catalyze specific chemical reactions. Moreover, platinum is used in dental alloys, spark plugs, sensors, turbine blade and biomedical applications. Moreover, it is proposed that Pt might be widely used to replace gold in electronic circuits (Gediga et al., 1998).

This chapter is aimed at

- Investigating the potential long-term impact of the worldwide increase use of platinum in fuel cell technology and other applications in terms of resources depletion
- Evaluating the long-term consequences of the worldwide increased demand of platinum on the cycles of other co-produced metals especially Ni and Cu

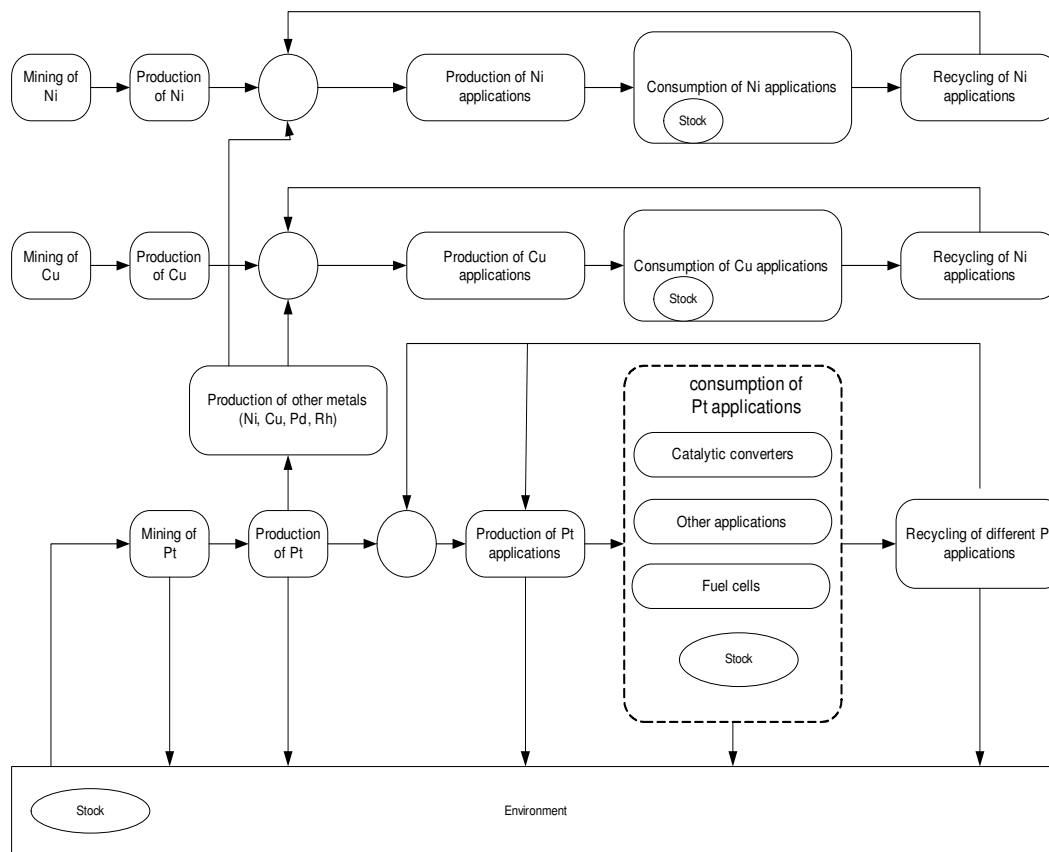
The analysis is carried out using a dynamic substance flow-stock model for platinum, nickel and copper, which is implemented in Matlab/SIMULINK environment (Math-Works, 2005).

The chapter is structured as follows. Section 2 outlines the general setup of the model. Section 3 contains the results of the model calculations and a discussion of the results. Section 4 is dedicated to the conclusions.



## 8.2 General setup of the model

The model described in this section is a dynamic substance flow-stock model. Figure 1 shows the modelled substances (platinum, nickel and copper), the main processes in their economic systems and their flows and stocks.



**Fig. 1:** The main processes in the economic system of Pt, Ni and Cu and their flows and stocks

The model includes the extraction of platinum, the production of platinum from primary resources and its main co-products, the production, consumption and waste management of platinum applications (fuel cell, catalytic converter, chemical industry, electrical and electronic industry, glass industry, investment, jewelry, petroleum industry and other applications) and the production of secondary platinum. The model also includes the production of co-produced metals (Ni and Cu) from primary resources, the consumption and waste management of Ni applications and Cu applications and the production of Ni and Cu from secondary resources.

Three types of platinum ores are identified, PGE dominants ores, Ni-Cu dominant ores and miscellaneous ores depending on the geographical distribution. Platinum resources in these ores can be classified as current reserve and identified resources. Current reserve includes all platinum resources that are economic to extract at current market price using existing technology. Identified resources include economic, marginally economic and sub-economic resources.

The demand in the model is the global demand for Pt, Ni and Cu and the supply of platinum is covered by four sources (Republic of South Africa, Russia, USA and Canada, and Other countries (Zimbabwe, Finland, China, Columbia and Australia)).

The model consists of a set of differential equations (Eqs. 1-6) describing the change of the magnitude of the substance stock in the system's compartments over time.

The change of the magnitude of the substance stock in the use phase over time is given by Eq. 1. The inflow into the stock-in-use is determined by external factors and the outflow is determined by the inflow, the product life span, and the emissions during use. The change of the magnitude of the substance stock in the production processes of platinum applications over time is given by Eq. 2 and equal to zero. The inflow into the stock is determined by the outflow from the stock, which is determined by the inflow into the stock-in-use. The change of the magnitude of the substance stock in the collection processes of platinum applications over time is given by Eq. 3 and equal to zero. The outflow from the stock is determined by the inflow into the stock, which is determined by the outflow from the stock-in-use. The change of the magnitude of the substance stock in the recycling processes of platinum applications over time is given by Eq. 4 and equal to zero. The outflow from the stock is determined by the inflow into the stock, which is determined by the outflow from the collection processes. The change of the magnitude of the substance stock in the mining processes of platinum over time is given by Eq. 5. The outflow from the stock is determined by the required primary platinum in the market. The change of the magnitude of the substance stock in the platinum market over time is given by Eq. 6 and equal to zero. The required platinum from primary resources (required to solve Eq. 5) is determined by the outflows from the recycling processes (estimated from Eq. 4) and the inflow of platinum into the production processes of its applications (estimated from Eq. 2)

Moreover, the model consists of several model relations describing the inflow of substances into the stock-in-use as function of the socio-economic variables. Some of the variables in the model relations constitute exogenous variables (GDP and population) and others are endogenous variables (price).

The historical data of the exogenous variables GDP and population size are given in Ayres et. al. (Ayres et al., 2003). In the future, GDP and population size are modelled as a function of time based on the historical data and the IPCC B1 Scenario for the future development in these variables.

The model also includes the environmental flows and stocks of platinum and an analysis of the energy required for the production of platinum, however these issues will not be discussed in details here.

$$\frac{dS_{x,C,i}}{dt} = F_{x,C,i}^{in}(t) - F_{x,C,i}^{out}(t) \quad (1)$$

$$\frac{dS_{x,PP,i}(t)}{dt} = 0 = F_{x,PP,i}^{in}(t) - F_{x,PP,i}^{out}(t) \quad (2)$$

$$\frac{dS_{x,SC,i}(t)}{dt} = 0 = F_{x,SC,i}^{in}(t) - F_{x,SC,i}^{out}(t) \quad (3)$$

$$\frac{dS_{x,R,i}(t)}{dt} = 0 = F_{x,R,i}^{in}(t) - F_{x,R,i}^{out}(t) \quad (4)$$

$$\frac{dS_{x,Res}(t)}{dt} = F_{x,Res}^{in}(t) - F_{x,Res}^{out}(t) = F_{x,Res}^{in}(t) - F_{x,Pr}^{in}(t) \quad (5)$$

$$\frac{dS_{x,m}(t)}{dt} = 0 = F_{x,R}^{out}(t) + F_{x,Pr}^{out}(t) - F_{x,PP}^{in}(t) \quad (6)$$

where  $x$ 's are the different metals (Pt, Ni, Cu),  $i$  is the metal application,  $C$  is the consumption of metal applications,  $PP$  is the production processes of metal applications,  $SC$  is the collection of the scrap of metal applications,  $R$  is the recycling of metal applications,  $Res$  is the identified resources of metals,  $M$  is the metals market,  $S$  is the stock,  $F^{in}$  is the inflow and  $F^{out}$  is the outflow.

### 8.2.1 Consuption of platinum applications

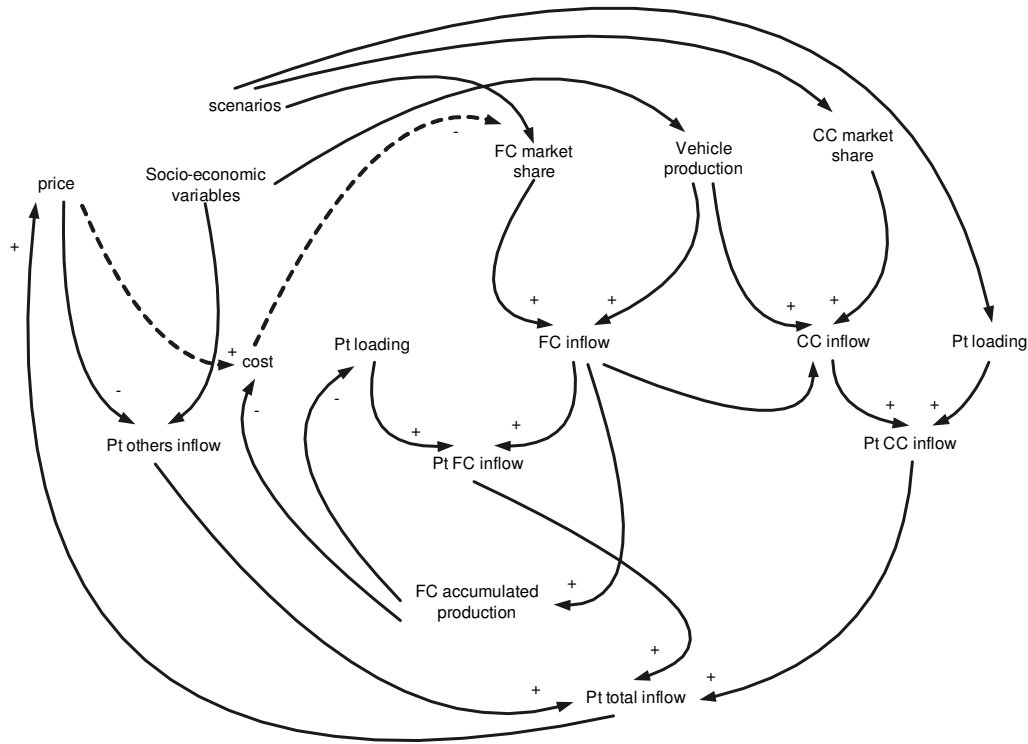
The change of the magnitude of the stock-in-use over time is the difference between the inflow and the outflow of platinum as given by the differential equation (Eq. 1).

#### *Inflow of platinum into stock-in-use*

The inflow of platinum into the stock-in-use is the amount of platinum used in catalytic converters, other applications and fuel cell and is modelled as given by Eq. 7. The relations between different factors determining the total inflow of platinum into the stock-in-use in the economic system are shown in figure 2.

$$F^{in}_{Pt,C}(t) = F^{in}_{Pt,FC}(t) + F^{in}_{Pt,CC}(t) + F^{in}_{Pt,Others}(t) \quad (7)$$

where  $F^{in}_{Pt,C}$  is the inflow of platinum into the stock-in-use,  $F^{in}_{Pt,FC}$  is the inflow of platinum into the stock-in-use of fuel cells,  $F^{in}_{Pt,CC}$  is the inflow of platinum into the stock-in-use of catalytic converters and  $F^{in}_{Pt,others}$  is the inflow of platinum into the stock-in-use of other applications.



**Fig. 2:** Total inflow of platinum into the stock-in-use model relations

The inflow of platinum into the stock-in-use of fuel cell is modelled based on the demand for vehicles, the share of fuel cell in the vehicles market and the platinum content of fuel cell as given by Eq. 8 and 9.

$$F^{in}_{FC,V}(t) = F^{in}_v(t) \cdot \lambda_{FC}(t) \cdot \left( \frac{T_v}{T_{FC}} \right) \quad (8)$$

$$F^{in}_{Pt,FC}(t) = F^{in}_{FC,V}(t) \cdot \alpha_{Pt,FC}(t) \quad (9)$$

where  $F_{FC,V}^{in}$  is the inflow of fuel cell in vehicles,  $F_v^{in}$  is the inflow of vehicles,  $T_v$  is the life span of vehicles,  $T_{FC}$  is the life span of fuel cell,  $F_{Pt,FC}^{in}$  is the inflow of platinum into the stock-in-use of fuel cells,  $\lambda_{FC}$  is fuel cell market share and  $\alpha_{Pt,FC}$  is the platinum content of fuel cell

The demand for vehicles is modelled based on socio-economic variables as given by Eq. 10.

$$F_v^{in}(t) = a + b \cdot GDP \quad (10)$$

Fuel cell market share ( $\lambda_{FC}$ ) is modelled based on different scenario using the following formula.

$$\lambda_{FC}(t) = \frac{100 \cdot e^{0.1(t-t_1)}}{1 + e^{0.1(t-t_1)}} \quad (\%) \quad (11)$$

The platinum content of fuel cell is modelled based on the learning curve concept. The learning curve (Tsuchiya & Kobayashi, 2004) is adapted for the possible reduction in platinum loading as given by Eq. 12.

$$\alpha_{Pt,FC}(t) = A \cdot X^{-r}(t) \quad (12)$$

$\alpha_{Pt,FC}(t)$  is the platinum loading of fuel cell at time t, A constant,  $X(t)$  cumulated production at time t.

The progress ratio  $F = 2^{-r}$

$$r = -\left[ \ln F / \ln 2 \right] \quad (13)$$

Although, the progress ratio may increase overtime for some technologies (Junginger et al., 2003), in the model the progress ratio is assumed to be constant during the simulation time.

For the recycling to be possible, the amount of platinum should not be lower than 20 g/FC. Therefore, the minimum Pt content in FC is set to 20 g in the model.

The inflow of platinum into the stock-in-use of catalytic converters is modelled based on the demand for vehicles as given by Eq. 10, fuel cell market share, catalytic converters market share and the platinum content of catalytic converters as given by Eq. 14, 15, 16 and 17.

$$F_{CC,V}^{in}(t) = \left[ F_v^{in}(t) - \left( F_{FC,V}^{in}(t) \cdot \left( T_{FC} / T_v \right) \right) \right] \cdot \lambda_{CC}(t) \cdot \left( T_v / T_{CC} \right) \quad (14)$$

$$F_{Pt,CC}^{in}(t) = F_{CC,V}^{in}(t) \cdot \alpha_{Pt,CC}(t) \quad (15)$$

$$\lambda_{CC}(t) = 100 \cdot \left( 1 - \left[ \frac{1}{e^{(t-t_0)/T_{CC}}} \right] \right) \% \quad (16)$$

$$\alpha_{Pt,CC}(t) = \text{stepfunction} \quad (17)$$

where  $\lambda_{CC}$  is catalytic converters market share and  $\alpha_{Pt,CC}$  is the platinum content of catalytic converters

As given by Eq. 16, the market share of catalytic converters is increasing over time, however, the number of vehicles occupied by catalytic converters is decreasing over time due to the impact of the introduction of fuel cell as given by Eq. 14.

The model assumes that at the time the vehicles are completely occupied by fuel cell (100% market share of fuel cell), the number of vehicles occupied by catalytic converters will be zero.

The inflows of platinum into the stock-in-use of other applications (chemical industry, petrochemical industry, glass industry, electrical and electronics industry, jewellery, investment and others (dental alloys, spark plugs, sensors, turbine blade and biomedical applications)) are modelled based on socio-economic variables such as per capita GDP (GDP and Pop), price and time. The socio-economic variables GDP, per capita GDP, and population size constitute exogenous variables and the price is an endogenous variable.

$$\ln[F_{Pt,i}^{in}(t)] = \beta_0 + \sum_{i=1}^n \ln[\beta_i X_i(t)] + \varepsilon(t) \quad (18)$$

$$\ln[P(t)] = \ln[a] + b \cdot \ln[D(t)] \quad (19)$$

### ***Outflow of platinum from stock-in-use***

The outflow of platinum from the stock-in-use of its applications is the outflow due to the discarded platinum products and the outflow due to the emissions during use.

$$F_{Pt,i}^{out}(t) = F_{Pt,E,i}^{out}(t) + F_{Pt,D,i}^{out}(t) \quad (20)$$

The emissions of platinum during the use phase of platinum applications are estimated as a fraction of the stock as given by Eq. 21.

$$F_{Pt,E,i}^{out}(t) = C_{Pt,i} \cdot S_{Pt,i}(t) \quad (21)$$

where  $C$  is the emission factor and  $S$  is the stock-in-use

The discarded outflow is estimated as a delayed inflow, corrected for the leaching that has taken place during use, as given by Eq. 22 and 23:

$$F_{Pt,D,i}^{out}(t) = F_{Pt,C,i}^{in}(t - L_{U,i}) - \sum_{i=1}^{L_U} C_{Pt,i} \cdot F_{Pt,C,i}^{in}(t - L_{U,i}) \cdot (1 - C_{Pt,i})^{i-1} \quad (22)$$

where  $F_{Pt,D,i}^{out}(t)$  is the outflow of application  $i$  due to the delay mechanism at time  $t$  and  $L_{U,i}$  being the average life span of the product in use.

$$F_{Pt,D,i}^{out}(t) = \sum_{j=0}^{\infty} W_j \cdot F_{Pt,C,i}^{in}(t - j) = \sum_{j=-\infty}^t W_{t-j} \cdot F_{Pt,C,i}^{in}(j) \quad (23)$$

where the lag weights  $w$ 's are the probabilities of exiting the delay in any time period  $j$  and must sum to unity

$$\sum_{j=0}^{\infty} W_j = 1 \quad (24)$$

The total outflow at time  $t$ ,  $F^{out}$  then is given by Eq. 25

$$F_{Pt,D}^{out}(t) = \sum_{i=1}^n F_{Pt,D,i}^{out}(t) \quad (25)$$

where  $F_{Pt,D}^{out}(t)$  is the total outflow due to the delay mechanism at time  $t$

### 8.2.2 Production of platinum applications

The change of the magnitude of the stock in the production of different platinum applications over time is the difference between the inflow and the outflow as given by the differential equation (Eq. 2).

#### *Inflow of platinum into production processes*

The input of platinum into the production processes of different platinum applications is equal to the output of platinum from the production processes in the products and the emissions during the production processes as given by Eq. 26.

$$F_{Pt,PP,i}^{in}(t) = F_{Pt,PP,i}^{out}(t) = F_{Pt,PP,P,i}^{out}(t) + F_{Pt,PP,E,i}^{out}(t) \quad (26)$$

#### *Outflow of platinum from production processes*

The output of platinum in the products is equal to the input of platinum into the stock-in-use as given by Eq. 27 and the emissions are estimated as a fraction of the input (Eq. 28).

$$F_{Pt,PP,P,i}^{out}(t) = F_{Pt,C,i}^{in}(t) \quad (27)$$

$$F_{Pt,PP,E,i}^{out}(t) = \beta_i \cdot F_{Pt,PP,i}^{in}(t) \quad (28)$$

From Eqs. 27 and 28, the inflow of platinum into the production processes

$$F_{Pt,PP,i}^{in}(t) = F_{Pt,C,i}^{in}(t) + \beta_i \cdot F_{Pt,PP,i}^{in}(t) = F_{Pt,C,i}^{in}(t) / (1 - \beta_i) \quad (29)$$

### 8.2.3 Production of platinum

#### *Secondary production*

The discarded outflow of platinum is either collected for recycling or ended up in the landfill sites and incineration plants. The collected flow for recycling is estimated as given by Eq. 30 and the landfilled and incinerated flows are estimated as given by Eq. 31.

$$F_{Pt,SC,i}^{in}(t) = \delta_i \cdot F_{Pt,D,i}^{out}(t) \quad (30)$$

$$F_{Pt,inc,land,i}^{in}(t) = F_{Pt,D,i}^{out}(t) - F_{Pt,SC,i}^{in}(t) \quad (31)$$

The change of the magnitude of the stock in the collection of different platinum applications over time is the difference between the inflow and the outflow and equal to zero as given by the differential equation (Eq. 3). Therefore, the inflow into the collection processes is equal to the outflow as given by Eq. 32.

$$F_{Pt,SC,i}^{in}(t) = F_{Pt,SC,i}^{out}(t) \quad (32)$$

The change of the magnitude of the stock in the recycling processes of different platinum applications over time is the difference between the inflow and the outflow as given by the differential equation (Eq. 4). Therefore, the inflow into the collection processes is equal to the outflow as given by Eq. 33.

$$F_{Pt,R,i}^{in}(t) = F_{Pt,R,i}^{out}(t) \quad (33)$$

The inflow into the recycling processes is equal to the outflow from the collection processes

$$F_{Pt,R,i}^{in}(t) = F_{Pt,SC,i}^{out}(t) \quad (34)$$

The outflow from the recycling processes is the refined platinum and the losses during the recycling processes (Eq. 35).

$$F_{Pt,R,i}^{out}(t) = F_{Pt,R,ref,i}^{out}(t) + F_{Pt,R,losses,i}^{out}(t) \quad (35)$$

The losses during the recycling processes are estimated as a fraction of the inflow into the recycling processes (Eq. 36).

$$F_{Pt,R,losses,i}^{out}(t) = \delta \cdot F_{Pt,R,i}^{in}(t) \quad (36)$$

The outflow (refined platinum) from the recycling processes (dismantling, smelting and refining) is estimated as given by Eq. 37.

$$F_{Pt,R,ref,i}^{out}(t) = F_{Pt,R,i}^{in}(t) \cdot (1 - \delta) \quad (37)$$

Total refined secondary platinum

$$F_{Pt,R,ref}^{out}(t) = \sum_{i=1}^n F_{Pt,R,ref,i}^{out}(t) \quad (38)$$

### **Primary production**

The required platinum from primary resources is estimated as the difference between the total demand for platinum and the possible supply of platinum from secondary resources as given by Eq. 39. The total extracted platinum from ores is estimated based on the required platinum from primary resources and the efficiency of the production processes (mining, concentration, smelting, base metal separation, and refining) of primary platinum efficiency as given by Eq. 40.

$$F_{Pt,pr}^{out}(t) = F_{Pt,PP}^{in}(t) - F_{Pt,R,ref}^{out}(t) \quad (39)$$

$$F_{Pt,pr}^{in}(t) = F_{Pt,pr}^{out}(t) \cdot (1 + \kappa) \quad (40)$$

$\kappa$  is the processes efficiency of primary platinum production

The losses during the production of primary platinum are estimated as give by Eq. 41.

$$F_{Pt,pr}^{losses}(t) = \kappa \cdot F_{Pt,Pr}^{in}(t) \quad (41)$$

### 8.2.4 Resources issues

The change of the magnitude of the stock of platinum resources over time is estimated in each country based on the required primary platinum and the possible increase of platinum resources as given by the differential equation (Eq. 5). The resources of platinum included in the model are the identified resources, which include the economic, marginally economic and sub-economic resources. The increase in the resources of platinum is assumed to be zero, therefore the change of the magnitude of the stock of platinum resources is estimated as given by 42.

$$\frac{dS_{Pt,Re s,A}(t)}{dt} = -F_{Pt,Re s,A}^{out}(t) = -F_{Pt,Pr,A}^{in}(t) \quad (42)$$

The supply of Pt from the main producing countries (Republic of South Africa, Russia, USA and Canada and other countries such as Finland, Zimbabwe, China, Columbia and Australia) is estimated based on an average value of the supply from these countries in the last 29 years and the total primary Pt required as given by Eq. 43.

$$F_{Pt,pr,A}^{in}(t) = \alpha_A \cdot F_{Pt,Pr}^{in}(t) \quad (43)$$

A in Eqs. 42 and 43 refers to the producing countries and  $\alpha_A$  is the supply from country A.

### 8.2.5 Co-production issues

Supply of co-produced metals as a result of Pt primary demand is estimated as given by Eq. 44.

$$S_{x,A}(t) = F_{Pt,pr,A}^{in}(t) \cdot \beta_{x,A} \quad (44)$$

$\beta_{x,A}$  is the concentration of specific co-produced material in the ore in specific country, x is the co-produced metals and A represents different countries

The total demand for different metal applications can either be estimated based on different scenarios or based on the socio-economic variables.

The total demand for metals ( $F_{x,C,total}^{in}$ ) are estimated based on socio-economic variables using Eqs. 18 and 19. The total inflow is divided into several applications based on the life span. Each one of these applications is estimated as given by Eq. 45.

$$F_{x,C,i}^{in}(t) = \chi_i \cdot F_{x,C,total}^{in}(t) \quad (45)$$

i represents the different products categories based on the life span

The change of the magnitude of the stock of the metals in the metals market over time is estimated based on the demand for the metals and the supply of these metals from primary resources and secondary resources as given by the differential equation (Eq. 6). Based on Eq. 6, the demand for the metals is equal to the supply of these metals from primary resources (from Pt ores and other ores) and the supply from secondary resources as given by Eq. 46.

$$F_{x,C}^{in}(t) = F_{x,R}^{out}(t) + F_{x,Pr,Pt}^{out}(t) + F_{x,Pr,other}^{out}(t) \quad (46)$$

$$F_{x,Pr,Pt}^{out}(t) = \sum_{i=1}^4 S_{x,A}(t) \quad (47)$$



The availability of the co-produced metals from secondary resources is estimated based on the discarded metals applications, the current collection rates and the efficiency of the recycling processes.

The discarded outflows of the metal applications are estimated based on their inflow and their life span as in a similar equation used for Pt applications (Eqs. 22-25).

The collected streams of co-produced metals applications are estimated based on the discarded outflow and the collection rate as given by Eq. 30.

The possibility of oversupply is checked by the estimates of the total demand for co-produced metals and the estimates of the supply of primary co-produced metals due to the demand for Pt. The required metals from other sources are estimated based on the difference between the total demand and the possible supply from Pt ores. The required amount of these metals from other sources (secondary sources and primary from other ores) is estimated as given by Eq. 48 and compared with the possible availability of metals from secondary resources.

$$F_{x,Pr,other}^{out}(t) + F_{x,R}^{out}(t) = F_{x,C}^{in}(t) - F_{x,Pr,Pt}^{out}(t) \quad (48)$$

## 8.3 Results and discussion

### 8.3.1 Platinum stock and demand

#### *Inflow of platinum into stock-in-use*

The total inflow of platinum into the stock-in-use is platinum inflow into the stock-in-use of its applications (fuel cell, catalytic converter and the other applications).

The inflow of platinum into the stock-in-use of fuel cell vehicles is estimated based on the demand for vehicles, market penetration of fuel cell vehicles and platinum required for each fuel cell. The demand for vehicles is modelled as a function of GDP, several scenarios are used for fuel cells market penetration and platinum required for each fuel cell is modelled based on the learning curve concept with initial loading of 60 g and a progress ratio of 0.97. Figure 3 shows the demand for platinum for fuel cell vehicles from 1975 through 2100 based on fuel cell vehicles market penetration scenarios. These scenarios are estimated as given by Eq. 11 to give values similar to those given by the UK department for transport (UK DFT, 2003) and listed in table 1.

**Table 1:** Scenarios used for fuel cell market penetration

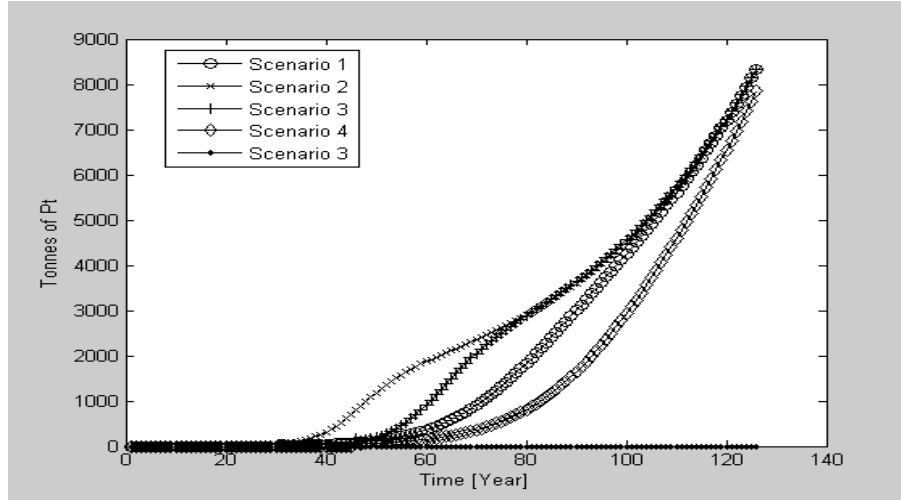
Scenario	2005	2020	2030	2040	2050	2070	2090	2100
Sc1	1	4.7	12	27	50	88	98	100
Sc2	3.5	50	90	99	100	100	100	100
Sc3	0	5	26	70	94	100	100	100
Sc4	0	2.4	5	10	20	53	84	100
Sc5	0	0	0	0	0	0	0	0

The amount of platinum required for each fuel cell over time is estimated as a function of the cumulated production of fuel cells based on the learning curve concept. Figure 4 shows the demand for platinum from 1975 through 2100 based on different progress ratios.

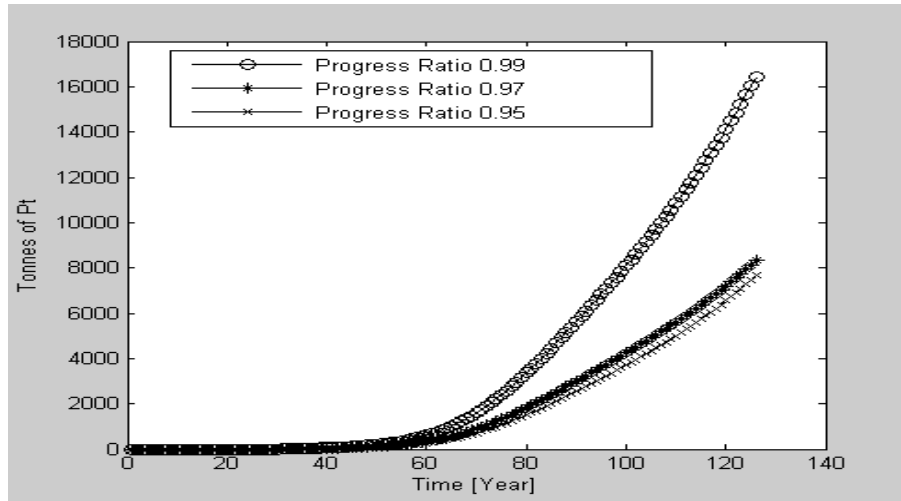
Although the amount of platinum required for one fuel cell is decreasing overtime reaching almost 20 g in 2100, the demand for Pt is increasing due to the increase demand for fuel cell vehicles. As shown in figure 2, the progress ratio is an important factor in determining the platinum content of fuel cells and consequently the total demand for Pt.

The inflow of platinum into the stock-in-use of catalytic converters is determined by the demand for vehicles, the market share of fuel cells, the market share of catalytic converters and the amount of platinum required for each catalytic converter as given by Eq. 14 and Eq. 15. The demand for vehicles is modelled as a function of the GDP as given by Eq. 10, the market share of catalytic converters is estimated based on scenario using Eq. 16 and Pt required for each catalytic converter is modelled as a step function taking the

value of 2 g from 1970 through 2005, 3 g from 2006 through 2012 and from 2013 onwards taking a maximum value of 4 g.



**Fig. 3:** worldwide platinum inflow into the stock-in-use of fuel cell vehicles under various scenarios regarding market penetration



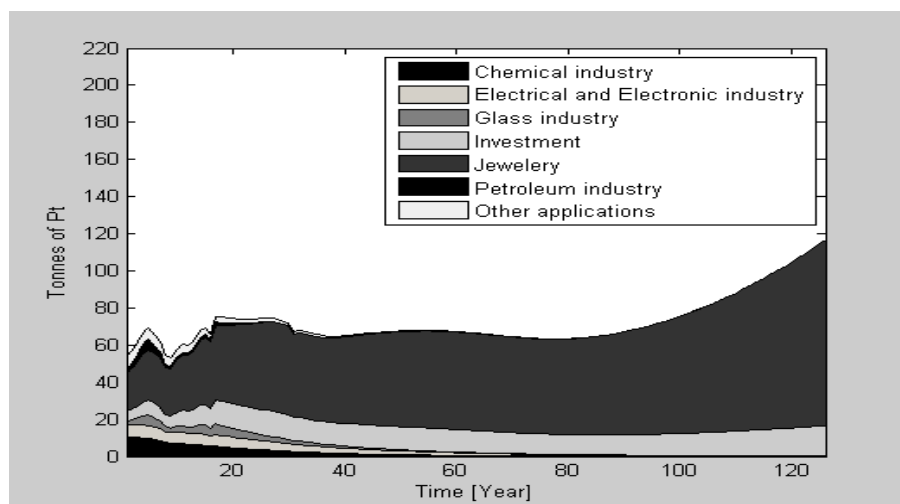
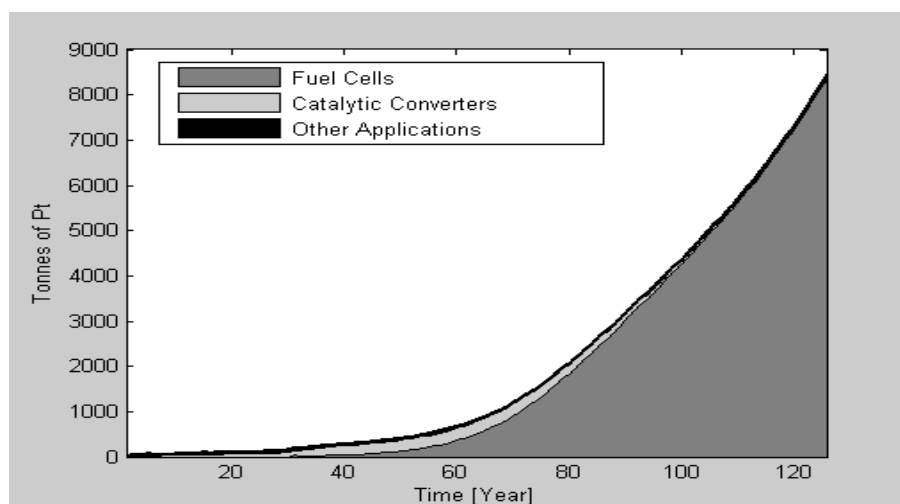
**Fig. 4:** worldwide platinum inflow into the stock-in-use of fuel cell vehicles under various assumption regarding progress ratios

The inflow of platinum into the stock-in-use of the other applications of platinum is modelled as a function of the GDP, platinum price and the time is used as a proxy of other determinants variables. Regression analysis is used to determine the relation between the explanatory variables and the inflow of platinum in each application. The model parameters and the goodness of the relations are shown in table 2. The analysis is carried out for the inflow from 1975 till 1990 (Johnson Mathey, 2005) . The inflows of these applications from 1975 through 2100 are shown in figure 5 and the total inflow of platinum into the stock-in-use of all applications from 1975 through 2100 is shown in figure 6.

Although the inflow of platinum into the stock-in-use of catalytic converters and some of the other applications is decreasing over time, the total demand for platinum is increasing due to the expected increase in demand for fuel cell vehicles and some of the other applications (jewellery and investment).

**Table 2:** Parameters used in modelling other applications inflows and the goodness of the relations

Application	a	b	c	d	R <sup>2</sup>
Chemical industry	1475.4	1.861	-0.081	-201.4	0.8
Petrochemical industry	13881.0	28.61	-0.054	-1943.6	0.45
Glass industry	7071.8	16.17	0.029	-989.5	0.64
Electrical and electronics industry	2229.8	4.917	-0.205	-312.9	0.68
Jewellery	1573.2	5.359	-0.582	-227.2	0.57
Investment	2888.8	8.494	-0.502	-413.43	0.19
Others	1312.4	1.098	-0.01	-177.1	0.84

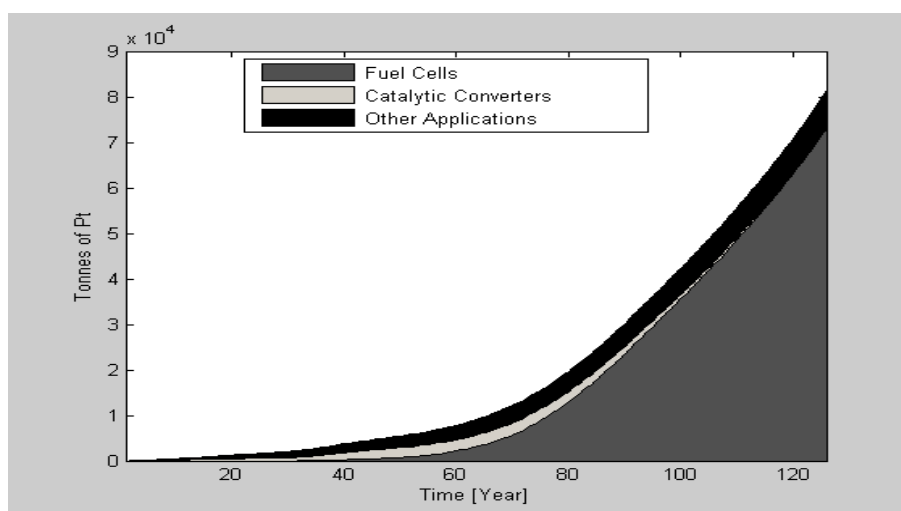
**Fig. 5:** The inflow of platinum into the stock-in-use of other applications**Fig. 6:** Total inflow of platinum into the stock-in-use of other applications, catalytic converters and fuel cells

The price of platinum is estimated as a function of platinum demand based on Eq. 19. The parameters  $a$  and  $b$  of this equation are estimated using regression analysis and their values are 12.1 and 0.942 consecutively. The outcome of the model shows that the increased demand for platinum caused an increase in the price of platinum and consequently a decrease in the demand in some of the other applications.

### ***Platinum stock-in-use***

The stock of platinum related to fuel cells, catalytic converters, and the other applications in the economic system is modelled from 1975 through 2100 based on Eq. 1 and shown in figure 7.

The stock-in-use of platinum in fuel cells is increasing over time. For catalytic converters, the stock-in-use is decreasing overtime due to the substitution by fuel cells reaching zero in 2100. The stock of other applications is increasing overtime, although it contributes only little to the total stock of Pt in use. The increase in the stock is mainly due to the increased demand for fuel cell vehicles and the life span of the fuel cell.



**Fig. 7:** Worldwide platinum in the stock-in-use of its applications

### ***Platinum losses***

The losses of platinum are due to the production of platinum from primary resources, the emissions of platinum during the production and consumption of catalytic converters and the waste management of platinum applications.

The emissions during use of platinum applications are estimated as a fraction of the stock in use as given by Eq. 21. The emission factor for catalytic converters (CC) is estimated using several parameters: the number of vehicles with CC, the average driving distance per vehicle, the emission per km, and the Pt loading. The emission factor is estimated for three countries, and the average is taken in the model. The parameters used in the estimates of the emission factor are listed in table 3a (Kummerer et al., 1999) and the emission factors for the three countries (Germany, Austria and The Netherlands) are listed in table 3b. The emission factors of the consumption of platinum applications and the production of catalytic converter are listed in table 3c. The losses of platinum in the production of platinum from secondary resources are estimated as given by Eq. 36 and the losses of platinum in the primary production are estimated as given by Eq. 41. The losses factors in platinum cycle are listed in table 4a (Hagelucken, 2003) and table 4b (Rade et al., 2001). The losses of platinum from 1975 through 2100 are shown in figure 8.

**Table 3a:** Parameters used in the estimates of the emission factors of catalytic converters\*

Parameters	D	A	NL
No of cars with CC	19200000	1607699	3307300
Driving distance (Km/car)	15000	14374	13580
Emissions ( $\mu\text{g/Km}$ )	0.65	0.5	0.5
Pt loading in CC (g/CC)	3	3	3

\* Kümmerer et al., 1999

**Table 3b:** Emission factors in some EU countries

Country	Emission factor
D	0.00325
A	0.0024
NL	0.0023
Average	0.00264

**Table 3c:** Emission factors of the consumption of platinum applications

Application	Emissions
Catalytic converter	0.0023
Electrical and electronic industry	0
Petrochemical industry	0.015
Glass industry	0.01
Others	1.0
Production of catalytic converters	0.01

**Table 4a:** Losses during the recycling of platinum applications\*

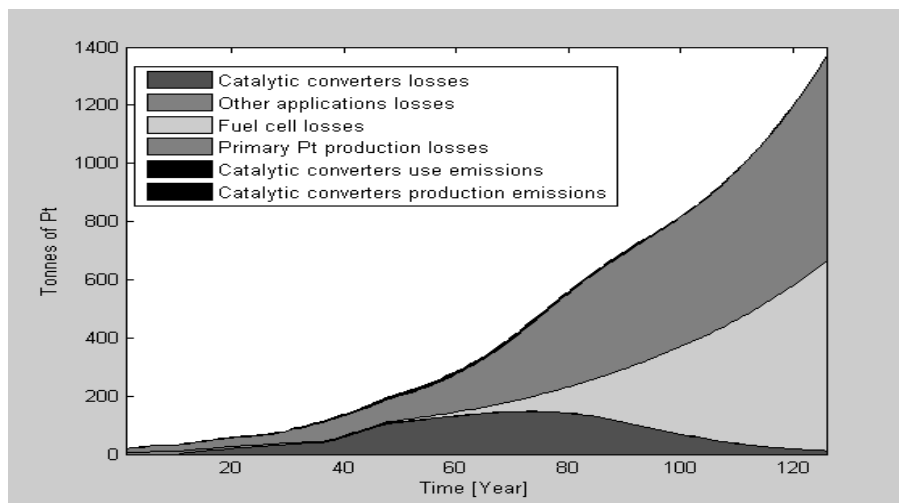
Application / processes	Losses %
<b>Fuel cell</b>	
Total recycling	10
<b>Catalytic converter</b>	
Dismantler	50
Collector	6
Decanner	3.2
Refiner	3.3
<b>Chemical industry</b>	
Refiner	6
<b>Electrical and electronic industry</b>	
Collection	50
Mechanical processes	20
Smelter	5
Refiner	1.05
<b>Petroleum industry</b>	
Refining	1.546
Refining	2.5
<b>Glass industry</b>	
Refining of spent GM equipments	1.01

\* Hagelucken C., 2003

**Table 4b:** Losses during primary platinum production \*

Processes	Losses %
Mining	10
Concentrating	10
Smelting	2
Refining	1

\* Rade et al., 2001

**Fig. 8:** Losses in platinum cycle

The emissions to the air due to the production and consumption of catalytic converter are small compared to the other losses, however, these emissions are expected to keep increasing till 2043 and decreasing afterwards. This trend is mainly due to the increase platinum content of catalytic converters and the declining market share of catalytic converters. These emissions amount to almost 503 tons in the period till the depletion of platinum resources.

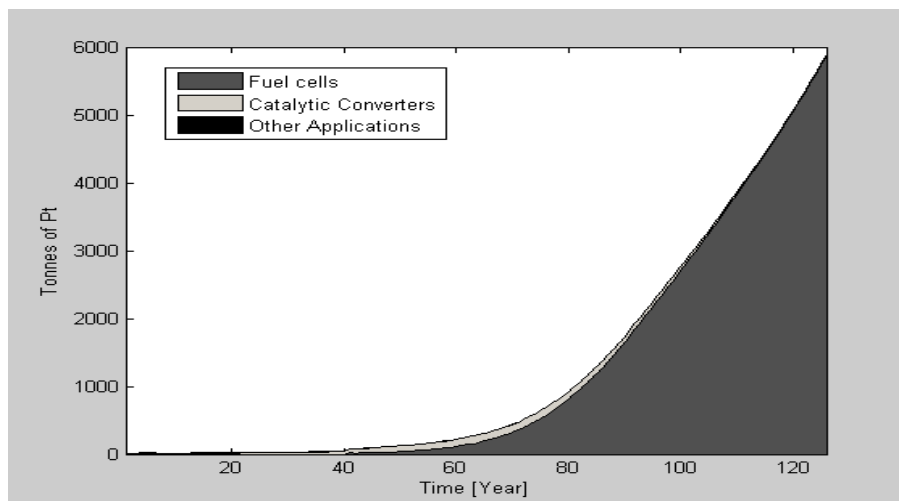
The losses of platinum due to the production of platinum from primary resources constitute the largest source of the losses and are increasing overtime. These losses amount to almost 11337 tons in the period till the depletion of platinum resources. The losses of platinum due to the waste management of catalytic converters are the second largest source. These losses are expected to increasing till 2047 and decreasing afterwards. These losses amount to almost 7044 tons in the period till the depletion of platinum resources. The losses of platinum due to the waste management of fuel cell are the third largest source and also increasing overtime. These losses amount to almost 2358 tons in the period till the depletion of platinum resources. The losses of platinum due to the other applications are decreasing overtime. These losses amount to almost 315 tons in the period till the depletion of platinum resources. The total losses of platinum is 21559 tons which is almost 43% of the total platinum identified resources

### 8.3.2 Platinum resources and primary and secondary supply

#### *Secondary supply*

The possible supply of platinum from secondary resources is estimated based on the discarded platinum applications and the efficiency of the recycling processes. The discarded platinum applications are estimated based on the past inflow and the life span of these applications. The life span of platinum

applications is listed in table 5 and the losses of platinum in the recycling processes are listed in table 4. The possible secondary supply of platinum from 1975 through 2100 is shown in figure 9.



**Fig. 9:** The possible worldwide supply of platinum from secondary resources

**Table 5:** Life span of platinum applications

Application	Life span (years)
Fuel cell	10
Catalytic converter	10
Electrical and electronics	5

The production of platinum from secondary sources is increasing overtime, however it covers only part of the total demand for platinum. The demand for platinum is increasing at higher speed. The percentage of the total demand for platinum, which is covered by secondary sources, is increasing overtime reaching about 70% at the end of the simulation time and about 55% at the time that platinum resources are depleted. The losses of platinum during the waste management of its application amount to 20% of platinum identified resources. These losses are mainly from catalytic converters and fuel cells. For both, the efficiency of the waste management could be increased.

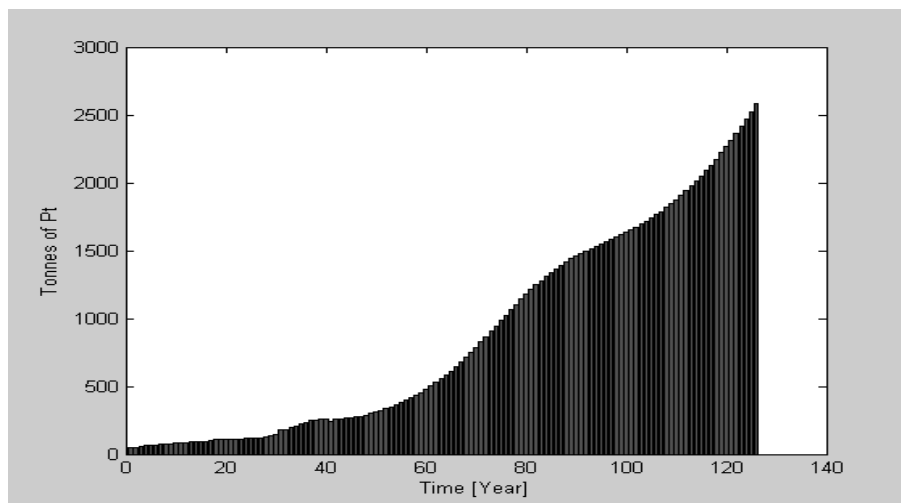
### **Primary supply**

Primary platinum required is estimated as the different between the total demand for platinum and the possible supply from secondary resources. The total demand for platinum is shown in figure 6, the possible supply from secondary resources is shown in figure 9 and the required primary platinum is shown in figure 10.

The required platinum from primary sources is increasing overtime. This is mainly due to the increase in platinum demand at a higher speed than the increase supply of platinum from secondary sources.

### **Resources of platinum**

At present, the required primary platinum is supplied mainly from South Africa and Russia. Small quantities are supplied from USA, Canada, and other countries. Platinum reserve (Blair, 2001) and identified resources (Vermaak, 1995) and the average supply of platinum of the last 29 years in the producing countries (Johnson Mathey, 2005) are listed in table 6. The total world identified resources of platinum as given by another reference is estimated as 47500 tons (Cawthorn, 1999)



**Fig. 10:** Platinum required from primary resources

**Table 6:** Platinum resources and the share in the world supply from different sites

Site	Resources (t0) tonnes	Reserve (t0) tonnes <sup>‡</sup>	Supply (%) <sup>†</sup>
RSA	31408	9437	74.95
RUS	3585	1417	17.85
USA & Canada	2027	283	5.3
Other	12287	3939	1.9
Total	49307	14538	100

\* Vermaak, 1995

† [www.Platinum.mathey.com](http://www.Platinum.mathey.com)

‡ Brad R. Blair, 2000

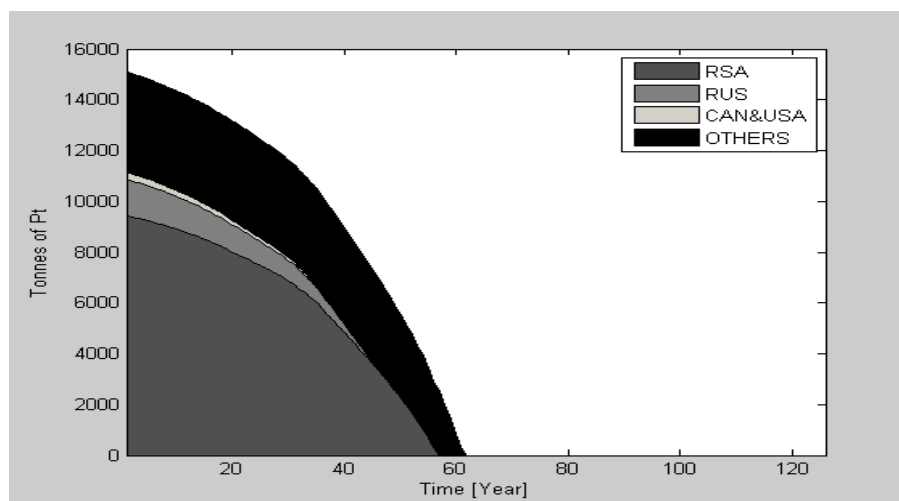
Due to the limited reserve and identified resources in the current supplying countries, in the future, the required primary platinum will be supplied mainly from other countries than those of today. The assumption in the model is that once the reserve or the identified resources of platinum is finished (i.e. the stock is reached zero) in a specific country, the model shifts the supply of platinum from this country to the other countries. Platinum current reserve and the identified resources of platinum in the producing countries are shown in figure 11 and 12.

As shown in figures 11 and 12, platinum current reserve will be depleted in three decades and the identified resources will be depleted in 2064. These estimates are based on the first scenario of fuel cell market penetration, progress ratio of 97%, fuel cell life span of 10 years and the losses in the waste management of fuel cell amount to 10 % of the total discarded outflow.

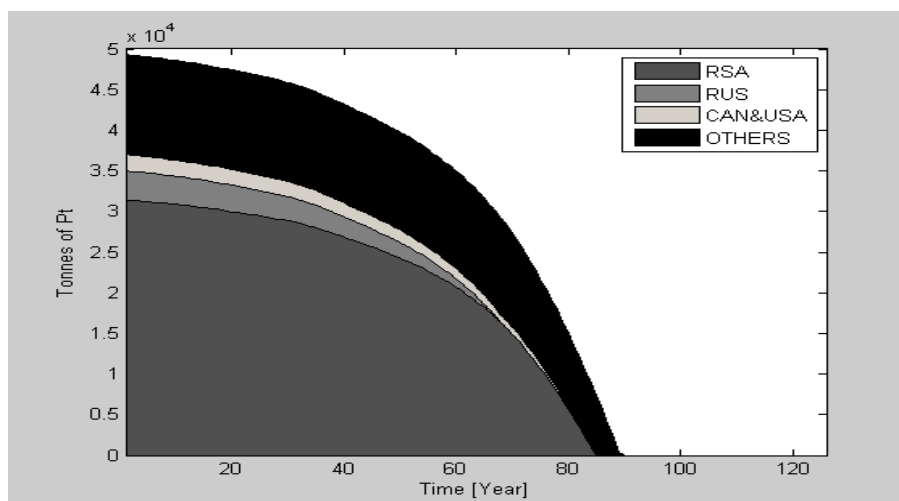
Although the platinum identified resources will be depleted in the world in 2064, a large amount of platinum will be accumulated in the economy by that time.

The model outcomes in terms of resources of platinum and co-produced Ni and Cu are sensitive to several parameters. These are the platinum content of fuel cell, platinum losses during the recycling processes of fuel cell and the fuel cell life span.





**Fig. 11:** Platinum current reserve in RSA, RUS, CAN, USA and Other Countries



**Fig. 12:** Platinum identified resources in RSA, RUS, CAN, USA and Other Countries

Table 7 shows the consequences of changing certain parameter on the depletion time of platinum identified resources.

The figures in the table show that the most important factor in determining the future availability of platinum resources are the progress ratio and the life span of fuel cells. The progress ratio influences the platinum content of fuel cell, which could minimize the total demand for platinum. An increase in the progress ratio of 2 % will lead to an increase of 9 years in platinum availability.

The fuel cell life span is an important factor in determining the time required for Pt to be depleted. Longer life span will make platinum available for longer time.

Although the decrease in the losses of platinum during the waste management of fuel cell will lead to an increase in the secondary supply of platinum, this will cover only small part of an increasing demand. Consequently it will increase platinum availability for short time.

Although based on the assumption made platinum will be exhausted in about 60 years from now, there are several possibilities for increasing the time before platinum is depleted.

If the fuel cell system is introduced gradually as it is in the forth scenario and the efficiencies of fuel cell production and waste management are increased (i.e. high progress ratio (increase by 2%) and low losses (decrease by 5%)) combined with an increase in the efficiency of the waste management of catalytic

converters mainly in the Dismantling process (increase by 30%), this will increase the availability of platinum by 13 years.

Moreover, there are other places for improvement such as the losses during the primary production of platinum and the possibility of collecting platinum from soil (Ely et al., 2001).

**Table 7:** The impact of different parameters on the platinum world identified resources

<b>Fixed Parameters</b>	<b>Scenario 1</b>	<b>Scenario 2</b>	<b>Scenario 3</b>	<b>Scenario 4</b>	<b>Scenario 5</b>
Progress ratio 97%	2064	2058	2058	2071	2088
Life span 10					
Recycling losses 10%					
	<b>Progress ratio 97%</b>	<b>Progress ratio 99%</b>	<b>Progress ratio 95%</b>		
Scenario 1	2064	2055	2067		
Life span 10					
Recycling losses 10%					
	<b>Life span 10</b>	<b>Life span 5</b>			
Scenario 1	2064	2059			
Progress ratio 97%					
Recycling losses 10%					
	<b>Recycling losses 10%</b>	<b>Recycling losses 5%</b>	<b>Recycling losses 15%</b>		
Scenario 1	2064	2065	2063		
Progress ratio 97%					
Life span 10					

### 8.3.3 Co-production of metals with platinum

The consequences of the introduction of fuel cells are not limited to the resource availability and other environmental impacts related to platinum cycle itself. It also has consequences in terms of the metals that are co-produced with platinum such as Ni and Cu.

The amount of metals co-produced with platinum is estimated based on Eq. 44 and the concentration of each metal in the ore in different producing countries as listed in table 8 (Athaus et al., 2003). The co-produced metals produced from platinum ores in South Africa is given in other sources as mining of 1 kg of Pt, yield 0.5 kg of Pd, 0.1 kg of Rh, 300 kg of Ni, and 200 kg of Cu (Pehnt, 2001).

Figure 13 shows the amounts of co-produced copper and nickel from 1975 through 2100 as a result of producing platinum from primary resources, considering the ore composition in the different producing countries.

The next step is comparing this supply with the worldwide demand for copper and nickel. The demand is estimated using different models for those metals. These models estimate the inflow of these metals into the stock-in-use of their applications, the outflow out of the stock through discarded products, and the amount of Cu and Ni available for recycling. The inflow into the stock, or in other words the demand, is modelled based on the socio-economic variables as given by Eqs. 18 and 19. The parameters in these equations are estimated using regression analysis. The analysis is carried out for the inflow from 1975 through 1990. The values of the parameters and strength of these relations are listed in table 9. The outflow of Cu and Ni with discarded products is estimated based on the past inflow and the life span of the metal applications.

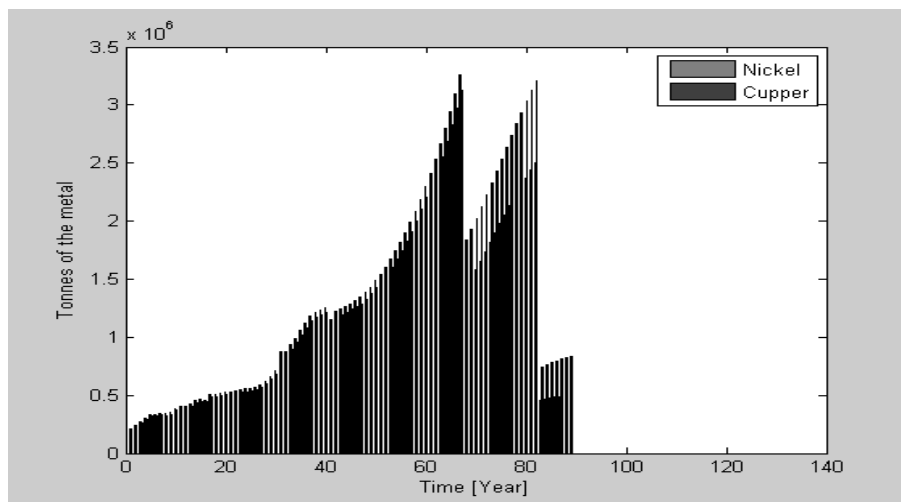
**Table 8:** Metals concentration in different platinum ores

Metal	Merensky RSA	UG2 RSA	Norilsk RUS	Stillwater USA	Sudbury Canada
Nickel (Ni) (%)	0.28	0.16	3.0	< 0.1	1.4-1.5
Copper (Cu) (%)	0.17	0.03	4.0	< 0.1	1.1-1.3
Platinum (Pt) (ppm)	4.82	3.22	2.5	6.0	0.38
Palladium (Pd) (ppm)	2.04	3.24	7.3	20.0	0.39
Rhenium (Rh) (ppm)	0.24	0.54	0.2	0.21	0.03

\* Athaus et al. 2003.

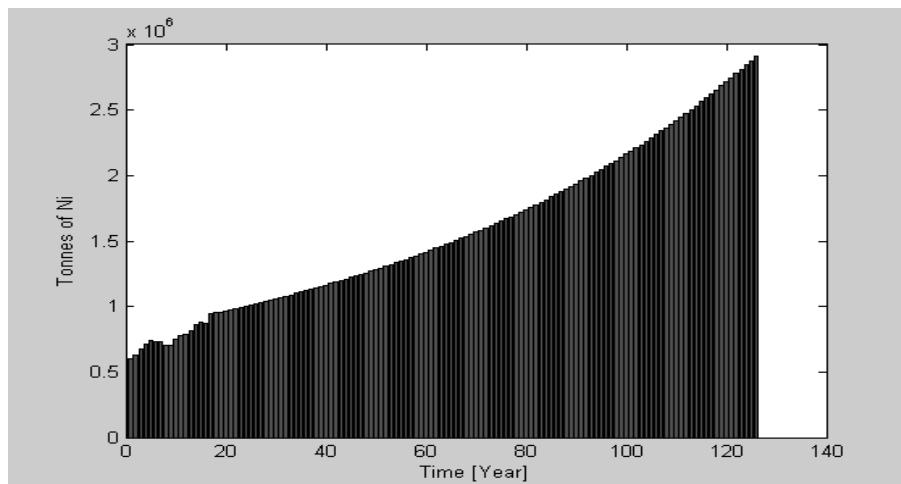
**Table 9:** Parameters used in modelling Nickel and Copper inflows and the goodness of the relations

Metal	A	b	c	d	R <sup>2</sup>
Nickel (Ni)	834.34	2.6334	-0.03194	-118.707	0.87
Copper (Cu)	1182.433	3.224	-0.0578	-166.58	0.93

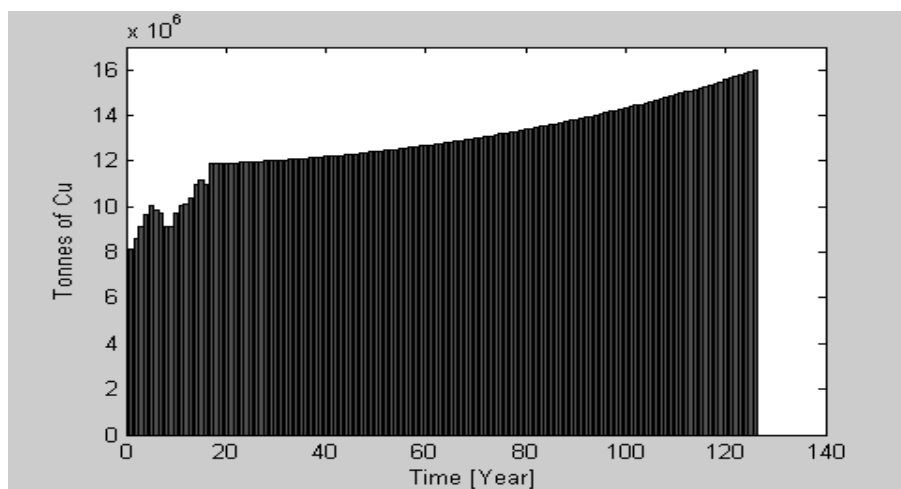
**Fig. 13:** Worldwide supply of Ni and Cu from Pt ores

The total demand for nickel and the total demand for copper from 1975 through 2100 are shown in figure 14a and 14b.

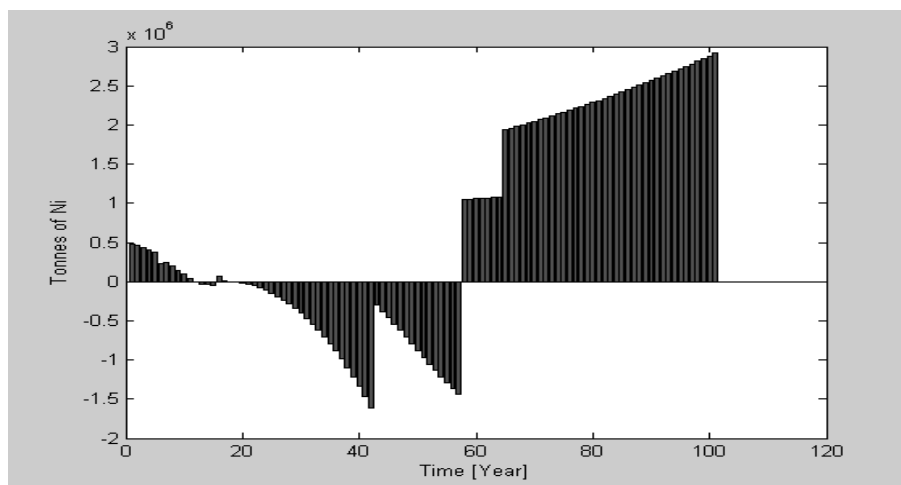
The demand for Ni and Cu is compared by the supply of these metals from Pt ores, and the difference is estimated as the required metals from other sources (primary and secondary) from 2000 through 2100 as shown in figures 15a and 15b.



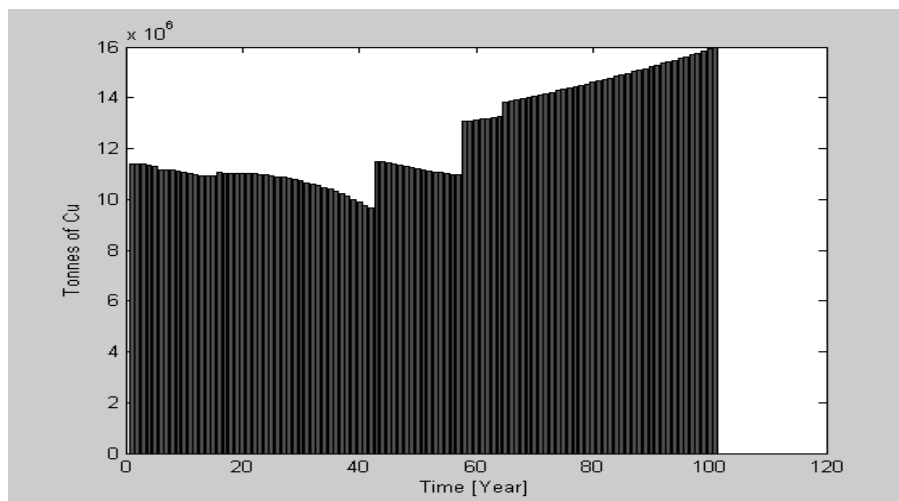
**Fig. 14a:** Worldwide inflow of Ni into the stock-in-use



**Fig. 14b:** Worldwide inflow of Cu into the stock-in-use

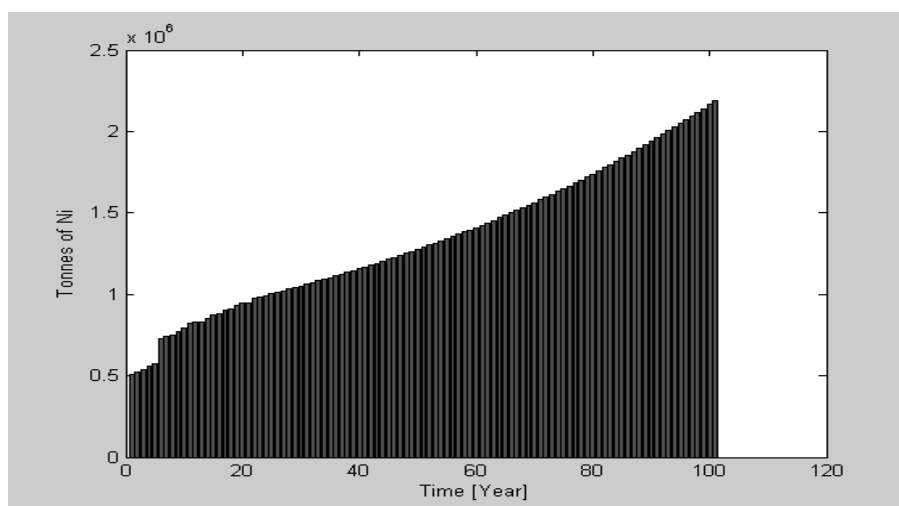


**Fig. 15a:** Ni required from other sources than those of Pt ores



**Fig. 15b:** Cu required from other sources than those of Pt ores

From these figures, we can see that for nickel, the supply from Pt ores is already quite high compared to the demand, at least until the moment the Pt ores are depleted. For copper, the demand is much higher, therefore the supply from Pt ores only covers a fraction. This implies that for Ni, the production from other sources including secondary sources will hardly be needed. This can have important consequences for both the mining and the recycling sector. The possible supply from secondary resources from 2000 through 2100, shown in figure 16, will not be needed until the moment the supply from Pt ores starts to decline.



**Fig. 16:** Worldwide secondary supply of Ni

The required Ni from other sources (primary and secondary) is compared with the possible supply from secondary resources. The results show that there is no need for Ni from primary resources for sometime after the Pt ores are depleted (i.e. secondary supply is enough to cover the demand). This means that if the primary production of Ni will continue after the Pt ores are depleted, the recycling of Ni will decline.

## 8.4 Conclusion

This chapter investigates the potential long-term impact of the increase use of platinum in fuel cell technology and other applications on platinum resources and evaluates the long-term consequences of the increased demand of platinum on the cycles of other co-produced metals especially Ni and Cu.

The model used in the analysis is a dynamic substance flow-stock model for platinum, nickel and copper and implemented in Matlab/SIMULINK environment.

The model estimates the development in platinum resources based on the global demand for platinum, the possible supply of platinum from secondary resources and the availability of platinum as identified resources in different producing countries.

The model estimates the development of the demand for the metals over time based on the development in the socio-economic factors. It estimates the possible supply of the metals from secondary resources based on the past inflow, the metal applications life span and the recycling efficiency. Moreover, it estimates the losses in the metals cycles.

The model shows that platinum resources will be depleted before the end of the century, however, there are a few factors may make platinum resources available for longer time.

The model shows that the most important parameters on the demand side are the efficiency of fuel cell production (indicated by the progress ratio) and the speed of fuel cell market penetration. An increase in the progress ratio of 2 % will lead to an increase of 9 years in platinum availability. This implies it is important to focus on technology development in this area.

The model also shows that the main platinum losses are due to the waste management of fuel cell and catalytic converters and the production of platinum from primary sources and constitute about 43% of the identified platinum resources at the time platinum resources are depleted.

On the supply side, the most important parameters are the efficiency of the waste management of fuel cell, the efficiency of the waste management of catalytic converters and efficiency of the production of platinum from primary sources. Another important factor is the life span of the fuel cell. The longer the life span, the longer platinum would be available.

The model shows that if the fuel cell system is introduced gradually (scenario 4) and the efficiencies of fuel cell production and waste management are increased (progress ratio increased by 2% and the losses decreased by 5%) combined with an increase in the efficiency of the waste management of catalytic converters (dismantling process efficiency increased by 30%), this will lead to an increase in the availability of platinum by 13 years.

Although the parameters in the model are affecting the availability of platinum, this effect is limited. This is mainly due to the growing demand for platinum, which is mainly driven, by the demand for vehicles and fuel cells that are increasing as long as the GDP is increasing.

Moreover, there are other places for improvement such as the losses during the primary production of platinum and the possibility of collecting platinum from soil.

The model also shows that the metals co-produced with platinum will be affected by the increased production of platinum. An increase in platinum production will lead to an increase in the production of co-produced metals. For the copper cycle, this will not have major consequences. Copper demand is very high compared to the supply from this specific source. For nickel, this is different: the supply of the metals from Pt ores exceeds its demand. This will have profound consequences for both mining and recycling of nickel.

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## **Chapter 9    Discussion, Conclusions and Recommendations**

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## 9.1 General discussion and evaluation of the case studies

The model developed and presented in this thesis is a dynamic substance flow-stock model that can be used to estimate future resource availability, emissions and waste streams. The model extends the currently available SFA models, firstly by combining flows and stocks, secondly by combining physical and economic elements, and thirdly by operating at two levels: of products, and substances.

This concluding chapter develops the discussion of a number of issues that were raised in chapters one to three of this thesis. These particularly pertain to a. the combination of flows and stocks, b. the combination of physical and economic elements, c. the level of scale in modelling substance flow and stocks, d. the inclusion of both the economic and the environmental subsystems, e. operating at two levels: products and substances and f. the role of uncertainty in dynamic substance flow-stock model.

In relation to the issue of the combination of flows and stocks, chapters one and two stated that several types of analysis are used to describe the relations between flows and stocks in the economic subsystem, including accounting and static and dynamic modelling (Van der Voet, 1996). The main difference between static and dynamic models is that the latter includes stocks within society (Bergbäck & Lohm, 1997), which play an important role in determining future waste and emissions of many hazardous substances to the environment and enable us to take into account the impact of delay, especially for applications with a long life span. Although the attention of those in the SFA community has been mainly focused on drawing up accounts and on comparative static modelling (Bringezu et al., 1997 and Bauer et al., 1997), a few specific substance stock databases or models have recently been published (Baccini, et al., 1996, Zeltner, et al., 1999, Kleijn, et al., 2000, Binder, 2001, Van der Voet, et al., 2002, Ayres, et al., 2003, Müller, et al., 2004, Spatari, et al., 2005, Binder et al., 2006). The model developed and presented in this thesis is a dynamic substance flow-stock model that consists of several sub-models. Each one consists of several substance flows and, in some cases, one or more stocks. In the chosen setup, the flows and stocks mutually influence each other: stocks are the result of flows while, at the same time, some of the flows are a result of the stocks. The main stock in the model is the stock-in-use. As stated in chapter 2, two different approaches can be used to model the stock-in-use, the inflow of substances into, and the outflow of substances from, the stock-in-use. The first approach starts from historical data on inflows and the product lifetime. The second approach starts from historic stock-in-use and the product lifetime. Although the first approach is the main one used in the model presented in this thesis, the second approach is also used, especially when statistical data on the inflow is lacking or where no correlation between the inflow and the socio-economic variables could be found. In general, the first approach leads to better estimates of the outflow of substances from the stock-in-use. This is mostly because the first approach directly estimates the outflow from the inflow, which is measurable. By contrast in the second approach, the outflow is calculated from an estimated stock. Other stocks of substances in the system also exist in the biosphere. For example, the geological stock which can be treated as the economic stock. The geological stock of substances used in the model (e.g. for platinum) includes both the currently known reserve and identified resources. Depending on the initial level of stock used in the model, the addition (inflow) to the resource stock can include newly found ores, or existing ores that become profitable. The extracted flow (the outflow from the resource stock) is mainly determined by the demand for the substance and the availability of secondary materials. The model does not contain mechanisms that describe the possible impacts of price increases or the development of new technologies in increasing the resource stock through making the currently known resource stock more profitable or making it feasible to extract lower-grade resources. However, these known (but unprofitable) resources are already included in the identified resources. The model also does not take into account the possibility of finding new ores, which might positively affect future resource availability. Future research may well focus on these issues.

With regard to the second point, of combining physical and economic elements into one model, chapter 2 stated that economic models usually ignore some crucial mechanisms, such as the physical laws of mass balance and stock building over time, that underlie the generation of waste and emissions (Van der Voet and Kleijn, 2000). On the other hand, material flow models limit themselves to physical considerations and do not include costs or incorporate mechanisms of economic analysis. The dynamic substance flow-stock model developed here is the first model in the field of substance and material flow analysis to combine elements from both types of models. In so doing the limitations of existing economic and material flow

models can be overcome and their strengths combined. The inclusion of economic elements in substance flow models enables coverage of a wide range of factors that affect the dynamic behaviour of the system, particularly in explaining the demand for products and, consequently, the demand for substances. The dynamics of the inflow and outflow of the substance in different phases of the economic subsystem are determined by distinct driving forces, implying the need to employ different explanatory variables in these sub-models. The socio-economic variables used in the model are: GDP, per capita GDP, sectoral share in GDP, population and material price. A time variable is used as a proxy for other determining factors. For lead, these variables were sufficient to explain a number of past trends in both intentional and non-intentional flows ( $R^2$  was between 0.34 and 0.95). However, the model forecasts are only valid assuming no unpredicted changes, such as the development of a completely new substitute. Although these explanatory variables proved to be the most influential ones other, more case-specific, variables could be also included in the analysis, subject to the availability of historic data and projections of the future development of these variables. For lead, the adopted explanatory variables did not appear to adequately describe a number of products, such as the flow of phosphate fertilisers and electricity production from coal. In modelling these flows time was used as a proxy of the effect of other influential variables. In the case of fertilisers other case-specific explanatory variables, such as the number of animals and agricultural yields, could also have been used in the analysis. However, these variables were not used in the Dutch case, as it is clear that the policy context is one of, if not the, most influential variables. Although the past use of coal for electricity production could not be directly explained by the explanatory variables, they were sufficient to describe total electricity production and the production of electricity from other sources and it was possible to use the production of electricity from coal as a balancing variable. Other general variables such as the general consumer price index (CPI) and the CPI for specific products could also have been used. This would have been especially useful in the absence of specific price information.

In relation to the third point, the level of scale in modelling substance flow and stocks, chapter 2 noted that substance flow analysis can be carried out at different levels: international, national, and local. The main issue regarding the level of scale is related to inclusion of economic elements in the model. If the modelled system is small (national or local), the components of the economic subsystem (extraction, production, consumption, and waste management) may be disconnected by trade (imports and exports of the refined substance, products containing the substance and obsolete products.). The smaller the country is, the stronger the disconnection will be. This disconnection does not exist if the system is modelled at the global level. In static substance flow analysis, it is sufficient to know the amount of imports and exports. However, in the dynamic substance flow analysis, knowing the amount of the imports and exports, or a time series of both, still requires the need to estimate both in the future and to arrive at an analysis of trade, using different explanatory variables. Most of the dynamic SFA models developed so far are either carried out on a global level (so imports and exports are not an issue) or do not take imports and exports into account, as in the model developed for copper in the USA (Zeltner et al. 1999). In the dynamic substance flow-stock model presented in this thesis, the import and export of products, obsolete products and refined substances are taken into account and treated as net imports that are estimated as a balancing item between two different components. This implies that information on past imports and exports are needed. For the future imports and exports are estimated together as one amount that its value could be positive or negative. It is not possible however to separate imports and exports and no analysis of trade can be made. This can be an issue for further research. This is the case for the lead model. Imports and exports at different stages in the economic subsystem of lead are treated as net imports to be estimated as a balancing item between two different components. This assumption is not needed in global models, such as the platinum case study in this thesis.

Regarding the fourth point, the inclusion of the economic and environmental subsystems, chapter 3 stated that the system in SFA is treated as a physical entity that consists of two subsystems, the economic and the environmental. However, sometimes, it is not clear where exactly to draw the border between the two. In the developed substance flow-stock models the economic subsystem includes extraction, production, consumption and waste management and the environmental components are restricted to air, water and non-agricultural soil. Agricultural soil may be seen as an environmental compartment, although the model treats it as part of the economic subsystem, as it is used as a means of production. Landfill sites are also treated as part of the economic subsystem, since in the Netherlands, at least, they are generally under human management. The choice of treating a landfill or agricultural soil as part of the environment or of

the economy does not make any difference in modelling terms or in the outcome of the SFA model. This is in contrast to, for example, LCA where the boundary between the technical subsystem and the environment has to be drawn as one of the system boundaries (Guinée et al., 1993) as this determines the classification of “emissions”. It is generally accepted that emissions from landfill sites should be included in the inventory and therefore, that landfill sites should be included in the technical subsystem (Heijungs et al., 1992 and Finnveden et al., 1995).

In most SFA studies the focus has been more on the economic subsystem (Zeltner et al., 1999, Graedel et al., 2002, Spataro et al., 2005), however some studies have placed more emphasis on the environmental subsystem (van der Voet, 1996, Guinée et al., 1999, Palm, 2002 and Tangsubkul et al., 2005). In principal, the level of detail required in including the environmental subsystem depends on the questions to be answered. Lead model includes detailed information about lead flows and stocks in the economic subsystem and environmental flows and stocks, which are directly linked to economic activities. The environmental components are generally treated as sinks (i.e. stocks with inflow but no outflow). Loops and cycles within the environmental subsystem are not included in detail. This level of detail is considered to be sufficient for estimating waste streams and emissions. The platinum model mainly focuses on the economic subsystem and includes the resource stock in the environment, which is sufficient to answer questions related to resource availability and the impact on the cycles of other metals.

To build a whole picture of the environmental flows and stocks and to analyse the potential risk that substances might cause, it is necessary to include environmental flows and stocks in detail. Future research may well focus on the detailed inclusion of the environmental subsystem and investigate the possibility of linking the flow-stock model with environmental models, such as environmental fate models and environmental risk assessment models.

In relation to the fifth point, operating at two levels (products and substances), chapter 3 stated that a stock of a substance or material is composed of all the products that contain the substance or material. This could include a large number of products, with greatly differing properties and behaviour. This implies that a substance stock model should contain at least two layers: the substance level and the product level. As stated in chapter 3, two approaches were used to model the inflow of substances into the stock-in-use. In the first approach (focused on products/substances), the inflow of substances is modelled on two equations; one describing the inflow of products and the other describing their substance content. Each one is determined by different factors. The inflow of products is determined by the socio-economic variables and the substance content is modelled either as a function of time or by using the learning curve concept, which introduces endogenous technical change into the model. Distinctions between these two levels have also been made in other system dynamic models (Meadows et al., 1972). In the second approach (focusing on substances), the inflow of substances into the stock-in-use is modelled directly by one equation, using different types of models. This approach is used when direct data is available about the substance level (i.e. the total amount of the substance used in the production of certain products). In this case, the explanatory variables used cover both the product inflow and substance content. The same approach has been used in modelling the demand for metals by using the Intensity of Use Technique (Tilton, 1990).

Operating at these two levels enables one to overcome the difficulties of modelling the substance stock-in-use. Often it is not possible to directly model this, because it consists of a large number of applications, each with different behaviour within the economic subsystem. Moreover, the approach also enables the inclusion of developments relating to both products and to substances and materials. Although the first approach has several advantages, the second approach is sometimes necessary as most data sources give direct information about the consumption of substances.

The general stock model, like many environmental or economic models contains several sources of uncertainty, of which three main types can be identified; disturbance (mainly arising from uncertainties in model inputs), perturbation (related to uncertainties about parameters in the model) and unknowable future inputs. In the dynamic substance flow-stock model there are several sources of uncertainty. The explanatory variables used in the model may be incomplete. Some variables may lose importance over time, while others may become more important. The approach used to estimate known flows and some of the parameters in the model's relations have been widely used in environmental and economic research. This approach has both advantages and limitations. The main limitation is future uncertainty. There is a basic assumption that the future relationship between the known flows and the socio-economic variables will be the same as it has been in the past. This is not always the case, as new developments may change

this relationship, such as the development of new materials or processes of production, use and waste management. Moreover, policy may also affect and change this relationship. The leaching model may contain uncertainties in the estimate of the annual loss fraction, which depend on many factors, such as the surrounding atmosphere, the weather, maintenance, and so on. In the delay model, the life span is always taken either as an average life span or as a life span distributed in time. The estimate of the former may be incorrect or liable to change over time. The chosen life span distribution or estimates for the minimum and maximum life span may also be inaccurate. Another possible source of uncertainty lies in the possibility of inaccurate estimates of the initial stocks.

Sensitivity analysis can be used in some of these parameters to evaluate the impact of possible changes on the model's outcome. Others, such as the initial stock of substances, will have a limited impact on the model's outcome. In the case of lead, the difference between the starting year of the past inflow and the starting year of future calculations exceeds the application's life span. For platinum, assumptions about the initial stock will not have any impact on the resource stock but may lead to an underestimate of the magnitude of the economic stock. In future research, comprehensive analysis of uncertainty is recommended.

## **9.2 Conclusions**

### **9.2.1 Methodology**

1. In order to estimate and compare the sources of problematic environmental flows, substance flow-stock model need to include both intentional and non-intentional applications of substances.
2. A substance flow-stock model should include both economic and physical-chemical variables. This is because substance flows through the economy are basically determined by economic demand for substance applications. Thus, in order to model them, the materials in which the substance occurs should be central modelling issue. In turn, substance flows out of the economy, in the shape of waste and emissions, are primarily determined by the physical-chemical properties of the substance.
3. A substance flow-stock model should include different factors or explanatory variables to cover different economic driving forces, such as the demand for the products containing the substance, the demand for secondary materials and policies on waste.
4. The use of the product/substance approach together with the use of the learning curve concept, which introduces endogenous technical change into the dynamic model of the substance content of products, will lead to better estimates of the demand for substances. Moreover, the inclusion of the stock-in-use and the hibernating stock will give better estimates of emissions and waste flows.
5. A substance flow-stock model can be used to evaluate the economic and environmental consequences of the presence of contaminants in products, by specifying the contribution of different applications to landfill or diffuse emissions over time. This is useful information for policies designed to prevent waste and pollution.
6. A substance flow-stock model can be used to improve the management of resources. It can do so by estimating the future availability of a substance for recycling, the future availability of primary resources and the future demand of the substance and substance containing applications. This is useful information for resource policy.
7. A substance flow-stock model can be used to evaluate technologies intended to promote sustainable production and consumption, at an early stage of their development.

### 9.2.2 Lead case study

8. The flows of lead through the economy are essentially determined by economic demand for its applications. Thus, the demand for lead can be modelled directly based on socio-economic variables, which appeared adequate in describing the historic demand for lead. This approach is only valid for future extrapolations if we assume that no unpredicted changes will occur.
9. The outflow of lead in the shape of solid waste and emissions is primarily determined by the physical-chemical properties of the substance. The main determinant factors are the life span of products, which are assumed to fit a Weibull distribution, and the emission factors.
10. The outcome of the model suggests that the amount of lead available for recycling in the Netherlands is expected to increase more than the demand for lead in the near future. This means that the demand for lead in the Netherlands can be met through the supply of secondary lead only. If comparable situations exist in other countries this may well have important consequences for the price of lead, on the profitability of primary production and the recycling industry. This might lead to an increase of landfilling and incineration at the expense of recycling, and thus to an increase of Pb emissions.
11. The environmental consequences of the non-intentional use of lead as part of zinc and iron ores and of coal are more severe than those originating from the waste streams of the intentional applications of lead and are considerable compared to those of lead intentional use. Non-intentional inflows of lead constitute less than 10% of the total lead inflow to the economy, but atmospheric emissions of lead from non-intentional applications are equal those from the intentional applications. Non-intentional flows of lead currently contribute 75% of the total amount of lead going to landfill and these are expected to rise to almost 90% of the total in the future.
12. It is expected that non-intentional flows of lead originating from the waste streams of intentional applications will decrease over time, due to more effective recycling. However, the overall flows of lead, as a contaminant in mixed primary resources, appear to be increasing.
13. The amount of lead from non-intentional sources is in principle sufficient to cover more than 10% of the total demand for lead. Therefore, the residues of production and consumption of non-intentional applications of lead can provide potential sources of lead, and other metals, in the future.
14. In terms of metals, the policy of increasing incineration of sewage sludge to minimise the amount of sludge going onto the land or being landfilled, will not be effective if the residues of incineration continue to be partly landfilled without the metals being removed..

### 9.2.3 Platinum case study

15. The use of a product/substance approach for fuel cells and catalytic converters, which constitute the biggest application of platinum, together with the use of the learning curve concept, which introduces endogenous technical change, combined with using the price as an endogenous variable would give better estimates of platinum demand.
16. The inclusion of the waste management phase of catalytic converters and other applications (in the chemical, electrical, electronic, glass and petroleum industries) in the platinum model would give better estimates of waste flows and help identify the main processes where improvements are needed.
17. Current reserves and identified resources of platinum will be depleted before the end of the century if no additional measures are taken.

18. There are a few factors on the demand and supply sides that may extend the availability of platinum, such as the increasing efficiency of fuel cell production, increases in the life span of fuel cells, their market penetration, increased efficiency in the waste management of fuel cells and catalytic converters and increasing efficiency of platinum production from primary sources.
19. If the fuel cell system is introduced gradually and the efficiency of production and waste management increases (efficiency of production increasing by 2% per year and losses decreasing by 5% per year) and there is an increase in the efficiency of the waste management of catalytic converters (dismantling process efficiency increasing by 30% per year), this will lead to an increase in the availability of platinum by 13 years.
20. The main losses of platinum are due to the waste management of fuel cells and of catalytic converters and to production of platinum from primary sources. At current rates of loss the accumulated platinum losses in waste stocks will constitute about 43% of identified platinum resources at the time platinum resources will be depleted.
21. Although the parameters in the model influence the assessment of the availability of platinum, this effect is limited. This is mainly due to the growing demand for platinum, which is mainly driven by demand for fuel cells. This in turn is driven by the demand for vehicles that increases in line with GDP.
22. The metals that are co-produced with platinum will be affected by increased platinum production, which will lead to an increase in the production of co-produced metals. The possibility of oversupply of the co-produced materials might have consequences in terms of their secondary production and their primary production from other sources. This will not have major consequences for the copper cycle as copper demand is much higher than the supply from this specific source. For nickel, however the story is different; as the supply of this metal from platinum ores is expected to exceed its demand, this will have profound consequences for both the primary mining and recycling of nickel.

## **9.3 Recommendations**

### **9.3.1 Methodological recommendations**

1. For forecasting purposes, existing substance flow models should be enlarged to substance flow-stock models in order to overcome the current limitation of forecasting models that are used to estimate solid waste flows and emissions, which are directly proportionate to the economic stock.
2. It is recommended that substance flow-stock models use different explanatory economic variables to cover the different driving forces. The use of more case specific explanatory variables, such as those mentioned for fertiliser flows in the lead case study, is also recommended.
3. It is recommended to study the development of stocks and flows of metals that occur naturally together in the same ores, as policies aimed at a specific metal could effect the cycles of other metals.
4. The development of user-friendly software that builds on the model developed for this thesis using MATLAB and SIMULINK is recommended.

### **9.3.2 Technical and policy recommendations**

1. Special attention should be given to the management of the non-intentional flows of lead, especially those originating from mixed primary resources containing lead as a contaminant (zinc and iron ores and coal).

2. It is recommended to recover the available metals contained in secondary materials, such as fly and bottom ashes generated from coal fired power plants and waste incineration plants, before landfilling or utilising them as construction materials. The removal of metals from residues generated by the incineration of sewage sludge is also recommended.
3. To increase the availability of platinum, it is important to focus on technology development in the area of fuel cell production. It is also important improve mining technologies to reduce the high losses in the production of platinum from primary resources. Moreover, a gradual introduction of fuel cell technology to the market is also recommended.
4. It is recommended to investigate the possibility of finding other sources of platinum supply. Platinum has been accumulating in the soil since the time that catalytic converters were first used. This could be a potential future source for platinum. Other sources include mixed primary resources.
5. In the long term, it is recommended to not use platinum for new purposes and to look for alternative technologies.

### **9.3.3 Specific recommendations for further research**

1. For future research, it is recommended to focus on the use of the substance flow-stock model in specific case studies related to the area of applications (waste prevention policy, pollution prevention policy, resource policy and technology assessment). Phosphorus is considered a scarce resource and is also a major cause of eutrophication, thus phosphorus management would make a good subject for a dynamic substance flow-stock model with useful implications for pollution and resource policy. Other possible case studies are the assessment of the impacts of the use of indium in solar cells, and electrical and electronic equipment waste (WEEE) management.
2. A further interesting topic for future research is the inclusion of mechanisms to describe the impact of price and technology development on the resource stock in the biosphere and the inclusion of an analysis of the impacts of energy use in the mining processes in the substance flow-stock model.
3. There are opportunities for enlarging the substance flow-stock model to include environmental flows in detail. This would improve estimates of the environmental concentration of substances in environmental media and assessment of their risks. In this respect it is important to investigate the possibilities of linking the substance flow-stock model to other environmental models, such as environmental fate models and environmental risk assessment models.
4. An interesting subject for future research is the inclusion of an analysis of trade in national substance flow-stock models.
5. To model the demand for substances, an approach based on modelling the inflow of substances into the stock-in-use as a function of the socio-economic variables is defined. A second possible approach could be based on estimating the inflow on basis of the substance's economic characteristics, that is, the functions that the substance fulfils in the products in which it is used. These economic characteristics strongly relate to the physical and chemical properties of the substance, which determine aspects such as durability, hardness, resistance to corrosion, protectiveness against radiation, flexibility, colour etc. These characteristics determine whether, or by which material, the substance in question can be replaced. This approach would enable the inclusion of substitution and technical developments in the model in addition to the already included socio-economic variables and remains an interesting issue for further future exploration.



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## Appendix

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## Appendix A - Additions to the regression analysis

### 1 Introduction

This appendix has a threefold aim. Firstly it gives an overview of more detailed statistical methods applied in regression analysis. Secondly it applies these methods to the results obtained in chapter 4. And thirdly, it performs a renewed more detailed analysis on the data of chapter 4.

Regression analysis is used in several scientific fields as a statistical tool to estimate and analyze the relation between a dependent variable and a number of independent, explanatory variables. Thus, regression analysis can for instance be used to describe the demand for electricity, metals or other commodities as a function of socio-economic variables such as GDP, population, price and further specific variables for any of these commodities (Liu et al. 1991; Labson and Crompton, 1993; Burney, 1995; Roberts, 1996; Moore et al. 1996; Ranjan and Jain, 1999; Guzman, et al. 2004; Mohamed and Bodger, 2005).

Regression analysis is used in this thesis for the analysis of the relative importance of different explanatory variables on the shape of the inflow of different metals; and subsequently on the stock-in-use over time. Regression analysis identifies the variables that are significant and contribute most to the dependent variable. It further examines the effect of separate significant variables, and also their combined effect. The fitting algorithm that determines the regression model parameters uses the ordinary least square (OLS) criterion (Gijbels and Rousson, 2001). The optimal regression model, the adequacy of the model and the significance of the variables are traditionally described in the following statistical parameters: the coefficient of determination ( $R^2$ ), the adjusted coefficient of determination ( $R^2_{adj}$ ), and the t- and F-statistics.

Although these statistical terms are normally used in the application of the regression model and in the determination of the significance of their individual variables, there are other statistical tests, which can be used to further examine the adequacy of the outcome of the regression analysis. This particularly pertains to the optimal number of explanatory variables, the degree of autocorrelation of the residues, the degree of multicollinearity and the assumption of homoscedasticity, that is, that the residuals do have a constant variance across observations. Below, these additional tests will be applied to the results of chapter 4.

In addition a new test round will be performed, using an adapted set of explanatory variables. The model presented in chapter 4 analyses the relation between the inflow of Cathode Ray Tubes (CRTs) into the stock-in-use as dependent variable and a number of socio-economic variables as explanatory variables. The socio-economic variables used are Gross Domestic Product (GDP), population size and time. These variables had been chosen on the basis of the above mentioned traditional statistical parameters: the coefficient of determination ( $R^2$ ), the adjusted coefficient of determination ( $R^2_{adj}$ ), and the t- and F-statistics.

Although in the analysis of Chapter 4, GDP and population size appeared to be the most influential variables and although this is also found in studies on other commodities (Liu et al. 1991 and Mohamed and Bodger, 2005), the inclusion of these variables in one model is questionable due to the high probability of multicollinearity between these two variables. This is the case because GDP is determined by the product of population size and welfare per capita. Therefore below a new analysis will be performed using population size and GDP per capita as explanatory variables.

In section 2 of this appendix a description will be given of the general aim and structure of regression analysis. In section 3 an overview will be given of the possibilities for more in depth testing the adequacy of the results of regression analysis. In section 4 these methods are applied to the results of chapter 4. In section 5, a renewed analysis will be performed, using other sets of explanatory variables. And in section 6 conclusions are drawn.

## 2 General aim and structure of regression analysis

### 2.1 Introduction

Regression analysis examines the strength of a relation between a dependent variable and a number of independent variables, also called explanatory variables. The mathematical model of the relation between the dependent variable and the explanatory variables is known as the regression model. The regression model contains one or more unknown parameters that are estimated using the given data on the explanatory variables. Eq. 1 describes the linear regression model that is used in the analysis:

$$Y(t) = \beta_0 + \sum_{i=1}^n \beta_i X_i(t) + \varepsilon(t) \quad (1)$$

where  $Y(t)$  is the inflow of product into the product stock at time  $t$ ,  $n$  is the number of explanatory variables,  $X_i(t)$  is the explanatory variables at time  $t$ ,  $\beta_i$  is the regression model parameter and  $\varepsilon(t)$  is the residuals of the regression model.

The fitting algorithm that determines the regression model parameters ( $\beta$ 's) in Eq. (1) uses the ordinary least square (OLS) criterion (Gijbels and Rousson, 2001). OLS is a mathematical optimization technique that attempts to find the best function that minimizes the sum of the squares of the residuals.

### 2.2 The coefficient of determination ( $R^2$ )

The coefficient of determination  $R^2$  is a non-dimensional measure of how well a regression model describes a set of data.  $R^2$  is a measure of how much of the variance in the dependent variable is explained by the explanatory variables in the regression model. Large values of  $R^2$  indicate better agreement between the model and the data. Eq. 2 gives the coefficient of determination ( $R^2$ ):

$$R^2 = \frac{SS_{reg}}{SS_{tot}} = 1 - \frac{SS_{res}}{SS_{tot}} \quad (2)$$

where  $SS_{reg}$  is the regression sum of squares,  $SS_{tot}$  is the total sum of squares and  $SS_{res}$  is the residuals sum of squares.

$R^2$  does not restrict the number of explanatory variables. Adding another explanatory variable (thus removing a degree of freedom) will always lead to an increase in the regression sum of squares ( $SS_{reg}$ ) (also called explained sum of squares) and a decrease in the residuals sum of squares ( $SS_{res}$ ), consequently an increase in  $R^2$ . Therefore  $R^2$  by itself is not a good indication for the most optimal regression model.

This problem can be solved by replacing the coefficient of determination ( $R^2$ ) by the adjusted coefficient of determination ( $R^2_{adj}$ ).

### 2.3 The adjusted coefficient of determination ( $R^2_{adj}$ )

The adjusted coefficient of determination ( $R^2_{adj}$ ) also describes the total explained variance by the explanatory variables but it penalizes adding too many additional variables (Glanz and Slinker, 1990). Therefore  $R^2_{adj}$  is used to find the optimal regression. Eq. 3 gives the adjusted coefficient of determination ( $R^2_{adj}$ ):

$$R^2_{adj} = 1 - \frac{MS_{res}}{MS_{tot}} = 1 - \frac{SS_{res} / (n - k - 1)}{SS_{tot} / (n - 1)} \quad (3)$$

where  $MS_{res}$  is the residuals mean squares,  $MS_{tot}$  is the total mean squares and  $k$  is the number of explanatory variables in the regression equation.

If another explanatory variable will be added, the number of explanatory variables ( $k$ ) will increase and the residuals sum of squares ( $SS_{res}$ ) will decrease. For  $R^2_{adj}$  to increase, the decrease in  $SS_{res}$  must be more than the decrease of  $(n-k-1)$ . The preferred model is the one with the highest  $R^2_{adj}$ .

## 2.4 t-statistics and F-statistics

The t-statistics indicates whether or not each regression parameters is significantly different from zero. The F-statistics indicates whether all explanatory variables taken together do significantly explain the dependent variable. Eq. 4 and Eq. 5 give the t-statistics and F-statistics. The critical values for t-statistics and F-statistics at different probability levels can be found in statistical books.

$$t = \frac{b_i}{Sb_i} \quad (4)$$

$$F = \frac{MS_{reg}}{MS_{res}} \quad (5)$$

where  $Sb_i$  is the standard error of  $b_i$  and  $MS_{reg}$  is the regression mean square

## 3 Possibilities for further analysis

### 3.1 Introduction

In addition to the above-mentioned statistical measures, there are other statistical tests that can be used for further examination of the adequacy of the regression model.

The first option for further improvement concerns the determination of the optimal regression model that is the optimal number of explanatory variables. For this reason Akaike's Information Criterion (AIC) and Schwartz Criterion (SIC) can be used. AIC is developed by Hirotugu Akaike in 1971. SIC, also called Bayesian information criterion (BIC) is developed by Schwartz in 1978. These two statistics have the same function as  $R^2_{adj}$  (Egelioglu et al. 2001 and Todeschini et al., 2004), but the SIC penalizes stronger for adding additional explanatory variables.

The second option concerns the determination of autocorrelation of the residuals from regression analysis. Autocorrelation of the residuals means that the model still can be improved and it leads to bias in the estimates of statistical significance of the parameters estimates. For this aim the Durbin – Watson Statistics, has been developed. Durbin – Watson Statistics is named after James Durbin and Geoffrey Watson.

Further points for improvement of regression analysis deal with the problem of multicollinearity and the problem of heteroscedasticity.

Multicollinearity refers to a high linear relationship between the explanatory variables used in the regression model. The best regression model is the model in which each of its explanatory variables correlates highly with the dependent variable but minimally with the other explanatory variables. Multicollinearity refers to a correlation between explanatory variables ( $R^2$ ) above 0.80. The problem associated with multicollinearity is the resulting overfitting in the regression analysis model. Multicollinearity however, does not affect the usefulness of a regression equation for purely empirical description of data or prediction of new observations if no interpretation is made based on the individual coefficient because multicollinearity problem does not result in biased coefficient estimates (Glanz and Slinker, 1990) but it increases the standard error of the estimates. Multicollinearity is a computational problem, that is, with existing perfect multicollinearity, the least square method can not be carried out (Makridakis et al., 1998). Therefore, most computer statistical software programs warn against serious multicollinearity (Glanz and Slinker, 1990).

Heteroscedasticity is a violation of the assumption that the residuals of the regression has a constant variance across observations (homoscedasticity). Also the violation of the assumption of homoscedasticity does not invalidate the regression model because the estimators remain unbiased and strongly consistent, but heteroscedasticity leads to an underestimation of the standard error thus deriving too narrow confidence intervals or small P-value (White, 1980 and Long and Ervin, 2000).

There are several methods that can be used to reduce the effect of heteroscedasticity (Long and Ervin, 2000 and Mackinnon and White, 1985) and with the advent of robust standard errors, testing conditional homoscedasticity is not as important as it used to be.

### 3.2 The optimal regression model

#### *Akaike's Information Criterion (AIC)*

Akaike's Information Criterion (AIC) as given by Eq. 6, can be used to find the optimal regression model.

$$AIC = 2k - 2\ln(L) \quad (6)$$

where k is the number of explanatory variables in the regression equation and L is the likelihood function.

Assuming that the model errors are normally distributed, Eq. 6 can be written as given by Eq. 7:

$$AIC = 2k - 2\ln\left(\frac{SS_{res}}{n}\right) \quad (7)$$

where n is the number of observations.

In the present equation the regression model will only be improved as long as AIC is decreasing. Therefore, the preferred model is the one with the lowest AIC value.

#### *Schwartz Criterion (SIC)*

Schwartz Criterion (SIC) as given by Eq. 8, can also be used to find the optimal regression model.

$$SIC = -2\ln(L) + k\ln(n) \quad (8)$$

Assuming that the model errors are normally distributed, Eq. 8 can be written as given by Eq. 9:

$$SIC = -2\ln\left(\frac{SS_{res}}{n}\right) + k\ln(n) \quad (9)$$

Comparable to above, SIC is decreasing as long as the regression model is improving by adding additional explanatory variables. The preferred model is the one with the lowest value of SIC.

### 3.3 Autocorrelation of the residuals

#### *Durbin – Watson Statistics*

Eq. 10 gives the Durbin – Watson Statistics. The value of Durbin-Watson statistics always lies between 0 and 4. Ideally, when there is no autocorrelation, the value of Durbin-Watson statistics should be close to 2. The critical values of Durbin – Watson Statistics, which are determined by the number of explanatory variables and the number of observations, can be found in statistical books.

$$d = \frac{\sum_{t=2}^T (e_t - e_{t-1})^2}{\sum_{t=1}^T (e_t)^2} \quad (10)$$

where  $e_t$  is the residuals associated with the observations at time  $t$ .

### 3.4 Multicollinearity

To test for multicollinearity, the correlation between the explanatory variables has to be checked. If the correlation between two explanatory variables is high, that is  $R^2$  higher than 0.80, the analysis is confounded by multicollinearity (Glanz and Slinker, 1990). This can be solved by a more careful selection or by redefinition of the explanatory variables, thus avoiding this problem.

### 3.5 Heteroscedasticity

Several tests can be used to examine heteroscedasticity such as Eyeball test, Breusch-Pagan test and others.

The **Eyeball test** is a graphic test used to test for heteroscedasticity by plotting the residuals of a regression model against one or more of the explanatory variables  $X$ 's or the predicted dependent variable  $Y$ . The assumption of homoscedasticity is not rejected if the dispersion of the residuals appears to be the same across all value of  $X$  or  $Y$ .

The **Breusch-Pagan test** is used to test for heteroscedasticity by testing whether the estimated residuals from a regression analysis is dependent on the values of the explanatory variables. The squared residuals is related to the explanatory variables. If the F-test confirms that the explanatory variables are jointly significant then the assumption of no heteroscedasticity is rejected.

## 4 Results of further elaboration of regression analysis of chapter 4

In this section, the results of the further analysis, using the above tests, of the CRT's inflow into the stock-in-use will be presented.

### 4.1 The optimal regression model

The explanatory variables used in the analysis are Gross Domestic Product (GDP), Population (Pop), and a Time variable (T). The time variable is used as a proxy for the combined influence of other variables on the inflow trend. The fitting algorithm that determines the regression model parameters ( $\beta_0, \beta_1, \beta_2, \beta_3$ ) in Eq. (11) uses the ordinary least square (OLS) criterion (Gijbels and Rousson, 2001).

$$Y(t) = \beta_0 + \beta_1 \cdot GDP(t) + \beta_2 \cdot Pop(t) + \beta_3 \cdot T(t) + \varepsilon(t) \quad (11)$$

where  $Y(t)$  is the inflow of goods at time  $t$ ,  $\beta_0$  is the overall mean response or regression intercept,  $\beta_1, \beta_2, \beta_3$  are the regression model parameters, GDP, Pop, and T are the explanatory variables and  $\varepsilon(t)$  is the residuals of the regression model.

Table 1 shows the result of the regression analysis, together with the results of the AIC and SIC statistics.



**Table 1:** Statistical analysis related to the regression analysis, using GDP, population and T as explanatory variables

Estimation	Socio-economic variables	$R^2$	$R^2_{adj}$	AIC	SIC	D/W	t-value	t-value	t-value	F-value
1	GDP	0.48	0.43	91.05	91.62	0.74	3.18			10.15
2	POP	0.68	0.65	84.70	85.26	1.06		4.84		23.49
3	Time	0.77	0.75	80.61	81.17	1.35			9.97	36.23
4	GDP, POP	0.70	0.64	86.02	87.15	1.24	-0.73	2.67		11.51
5	POP, Time	0.82	0.79	78.94	80.07	1.71		-1.80	2.85	23.46
6	GDP, Time	0.78	0.73	82.13	83.26	1.48	-0.61		3.63	17.27
7	GDP, POP, Time	0.85	0.80	78.64	80.34	2.07	1.32	-2.17	3.08	17.38

$R^2$  is used in the analysis as indication of the model that gives maximum explained variance by the explanatory variables independent of the number of these variables. It is clear from Table 1 that the maximum  $R^2$  ( $R^2 = 0.85$ ) was obtained when the three explanatory variables are included in the regression model (estimation 7).  $R^2_{adj}$  is similar to  $R^2$  but it reaches the maximum with the optimal number of explanatory variable. The maximum  $R^2_{adj}$  ( $R^2_{adj} = 0.80$ ) was also obtained when the three variables are included in the regression model. The t-statistics for the individual coefficients shows that in this model the GDP and population are not significant. However, the F-statistics indicates that all the three explanatory variables taken together are significant and contribute to the inflow. Therefore the optimal model is the model that includes the three explanatory variables GDP, population and time.

## 4.2 Further tests for the optimal regression model

The optimal model in chapter 4 is determined using  $R^2_{adj}$ . Other tests comparable to  $R^2_{adj}$  can also be used to find the optimal model such as the AIC and SIC tests. The SIC test however, penalizes adding additional variable more than the AIC test. It is clear from estimation 7, when the three variables are included in the regression model, that the AIC has the lowest value. With respect to the SIC test, the results show that SIC has the lowest value when two variables are included in the model (estimation 5), however it is only slightly lower than the one associated with estimation 7. Therefore, with the given set of explanatory variables, the best model is the one that includes GDP, population and time as explanatory variables.

## 4.3 Autocorrelation of the residuals

The Durbin – Watson Statistics, also presented in table 1, shows no autocorrelation of the residuals from regression analysis. So the estimates of statistical significance of the parameters are not biased.

## 4.4 Multicollinearity

The explanatory variables in the chosen model are tested for multicollinearity. The correlation between the GDP and time is 0.69, and the correlation between the POP and GDP is 0.80. Both values are not above the limit value set for multicollinearity. Therefore, the multicollinearity problem does not exist in the model when GDP, population and time are used.

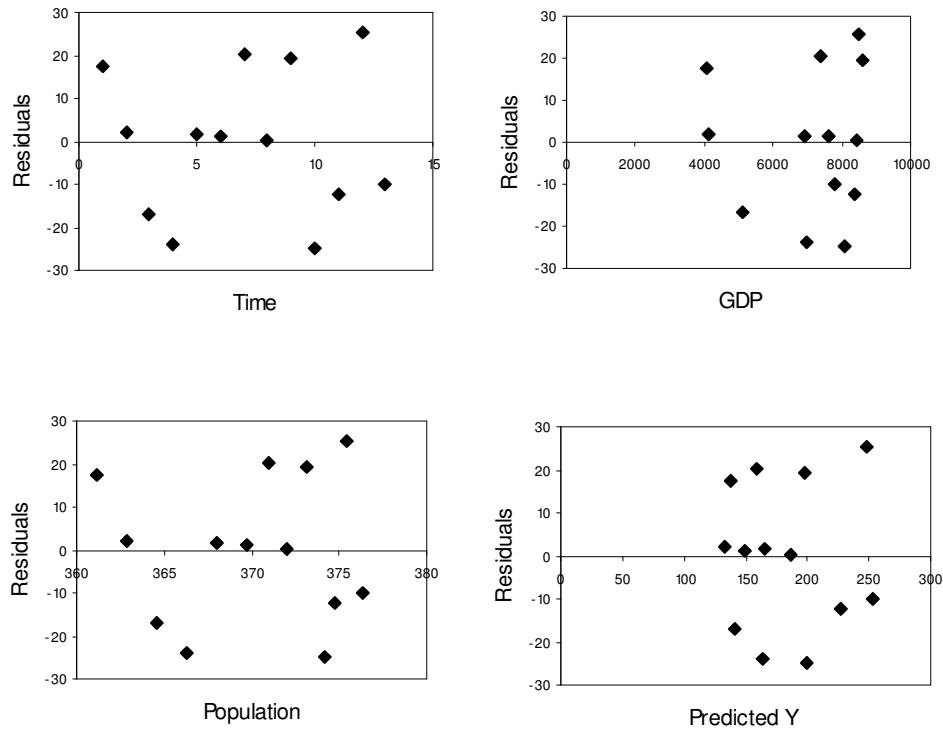
## 4.5 Heteroscedasticity

The chosen model is tested for heteroscedasticity using the Eyeball test and Breusch-Pagan test. The Eyeball test is used to examine the regression model, including the GDP, population and time, for heteroscedasticity. The residuals of the regression model are plotted against the explanatory variables and the predicted value of the inflow. The results are shown in figure 1.

The variability of the residuals appears to be the same across all values of the explanatory variables and of the predicted inflow. It is known that the dispersion of the residuals is increasing if the values of the explanatory variables and of the predicted dependent variable Y are increasing when heteroscedasticity

does exist; in the present model this is not the case. Therefore the assumption of homoscedasticity is not rejected.

The regression model is also tested for heteroscedasticity using the Breusch-Pagan test. The squared residuals are related to the explanatory variables (GDP, population and time). The F-test with a value of 0.26 indicates that all the explanatory variables taken together are not significant. The F-test confirms that the explanatory variables together is not significant, therefore the assumption of no heteroscedasticity is not rejected.



**Fig. 1:** Plot of the residuals of the regression model against the explanatory variables using the Eeyball test

## 5 Results when using per capita GDP (GDP/C) as explanatory variable

### 5.1 The optimal regression model

In this section a new analysis will be performed, based on a more strict preselection of explanatory variables aiming at avoidance of correlation between explanatory variables. More specifically, GDP is replaced by GDP per capita (GDP/C), thus avoiding overlap with POP. The results of the statistical tests when GDP/C is used in the analysis are presented in table 2.

**Table 2:** Statistical analysis using GDP/C, population and T as explanatory variables

Estimation	Socio-economic variables	$R^2$	$R^2_{adj}$	AIC	SIC	D/W	t-value	t-value	t-value	F-value
1	GDP/C	0.46	0.41	91.54	92.11	0.71	3.06			09.37
2	POP	0.68	0.65	84.70	85.26	1.06		4.85		23.49
3	Time	0.77	0.75	80.61	81.17	1.35			6.02	36.24
4	GDP/C, POP	0.70	0.64	86.01	87.14	1.24	-0.74	2.80		11.53
5	POP, Time	0.82	0.79	78.94	80.07	1.71		-1.80	2.86	23.47
6	GDP/C, Time	0.78	0.73	82.17	83.30	1.47	-0.59		3.74	17.21
7	GDP/C, POP, Time	0.85	0.81	78.53	80.22	2.09	1.36	-2.21	3.11	17.56

It is clear from the estimation 7 in Table 2 that when all the three variables are included in the regression model, not only  $R^2$  but also  $R^2_{adj}$  has the highest value ( $R^2 = 0.85$  and  $R^2_{adj} = 0.81$ ). Comparably, AIC has the lowest value in estimation 7. SIC still has its lowest value in estimation 5 with two explanatory variables. The t-statistics for the individual coefficients shows that in this model the GDP/C and population are not significant. However, the F-statistics indicates that all the three explanatory variables taken together are significant and contribute to the inflow. Therefore the model with three explanatory variables is still the optimal model.

If the results of the model that includes GDP/C are compared with the results of the model, which includes GDP as explanatory variable, we can observe that the use of GDP/C gives slightly better results. However there is no big difference between the two models.

### 5.2 Autocorrelation of the residuals

The Durbin – Watson Statistics in table 2 shows that there is no autocorrelation in the residuals of regression analysis. So the estimates of statistical significance of the parameters are not biased.

### 5.3 Multicollinearity

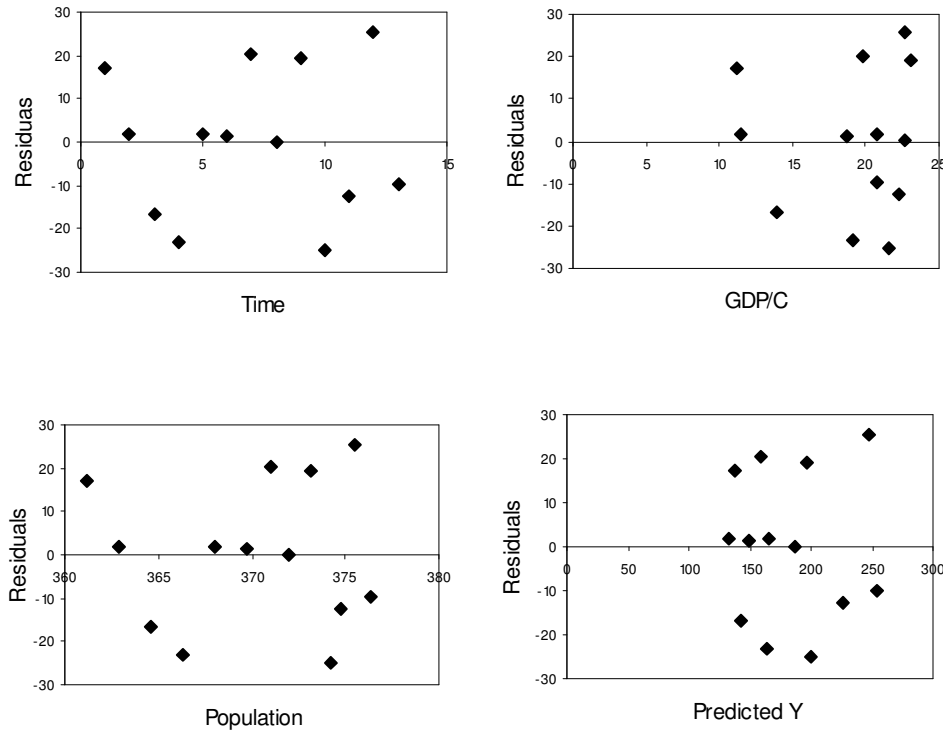
The explanatory variables in the chosen model are tested for multicollinearity. The correlation between the GDP/C and time is 0.66, and the correlation between the POP and GDP/C is 0.77, therefore, the multicollinearity problem does not exist in the model.

### 5.4 Heteroscedasticity

The chosen model is tested for heteroscedasticity using the Eyeball test and Breusch-Pagan test.

The results of the Eyeball test are shown in figure 2. The variability of the residuals appears to be the same across all values of the explanatory variables (GDP/C, population and time) and the predicted dependent variable (inflow of CRTs). So also here the assumption of homoscedasticity is not rejected.

When using the Breusch-Pagan test, the F-statistics shows a value of 0.26, which indicates that all the explanatory variables taken together are not significant. The F-statistics confirms that the explanatory variables are jointly not significant, therefore the assumption of no heteroscedasticity is not rejected.



**Fig. 2:** Plot of the residuals of the regression model against the explanatory variables, when using GDP/C instead of GDP in the regression model

## 6 Conclusions

The statistical methods presented in this appendix are more elaborate than those used in chapter 4. However, there appears to be no change in the general conclusions drawn from the regression analysis. The best model is the one that includes GDP (or GDP/C), population and time as explanatory variables.

The results of the additional statistical tests in this appendix did validate the results of this model. The multicollinearity problem does not exist in the model. There appears to be no autocorrelation of the residuals from the regression analysis. And the assumption of homoscedasticity is not rejected. Thus the model including the three explanatory variables can be used.

Although the results obtained when GDP/C is used in combination with other explanatory variables in the regression model appeared to be slightly better than those when GDP is used, there is no big difference between the outcomes of the two models. Therefore the results of chapter 4 still hold.

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## Appendix B – List of symbols in the thesis

### Appendix B 1 – List of symbols in chapter 3

$F_{PC,i}^{in}$  is the inflow of a product into the  $i$ th product stock.  
 $F_{C,i}^{in}$  is the inflow of the substance into the  $i$ th product stock.  
 $SC$  is the substance content.  
 $F_C^{in}$  is the total inflow of the substance into the consumption phase.  
 $F_{C,E,i}^{out}$  is the outflow of the substance in the  $i$ th product due to emissions.  
 $F_{C,D,i}^{out}$  is the outflow of the substance in the  $i$ th product due to the delay mechanism.  
 $S_{C,i}$  is the stock-in-use of the substance in the  $i$ th product.  
 $F_H^{in}$  is the inflow of the substance into the hibernating stock.  
 $F_H^{out}$  is the outflow of the substance from the hibernating stock.  
 $F_P^{in}$  is the input of the substance into primary production processes (the extracted flow).  
 $F_P^{out}$  is the outflow of the substance from primary production processes (refined primary substances).  
 $F_X^{in}$  is the inflow of the co-produced substances into the economy.  
 $F_{PP}^{in}$  is the total inflow of the substance into the production processes of all applications.  
 $F_{PP,i}^{in}$  is the inflow of the substance into the production process of the  $i$ th product.  
 $F_{PP,i,P}^{out}$  is the outflow of the substance in the produced  $i$ th product.  
 $F_{PP,i,A}^{out}$  is the outflow of the substance to the air during the production process of the  $i$ th product.  
 $F_{PP,i,W}^{out}$  is the outflow of the substance to the water during the production process of the  $i$ th product.  
 $F_{PP,i,L}^{out}$  is the outflow of the substance to landfill sites from the production process of the  $i$ th product.  
 $F_{SC,i}^{in}$  is the amount of waste collected for recycling purposes.  
 $F_{inc,land,i}^{in}$  is the inflow of the substance into incineration plants and landfill sites from the discarded  $i$ th product.  
 $F_{inc,DC,i}^{in}$  is the inflow of the substance into incineration plants from the discarded  $i$ th product.  
 $F_{land,DC,i}^{in}$  is the inflow of the substance into landfill sites from the discarded  $i$ th product.  
 $F_{SC,i}^{out}$  is the outflow of the substance from the collection phase.  
 $F_{SC,i,E}^{out}$  is the emitted outflow from the collection phase.  
 $F_{SC,i,R}^{out}$  is the outflow which goes to the recycling processes.  
 $S_{sc}$  is the stock of the substance in the collection phase.  
 $F_R^{in}$  is the inflow of the substance into recycling processes  
 $F_R^{out}$  is the total outflow of the substance from recycling processes.  
 $F_{R,E}^{out}$  is the emitted outflow of the substance.  
 $F_{R,W}^{out}$  is the landfilled outflow of the substance.  
 $F_{R,CNI}^{out}$  is the waste outflow used in other applications (non-intentional applications).  
 $F_{R,R}^{out}$  is the outflow of the refined substance from recycling processes.  
 $F_{inc,t}^{in}$  is the total inflow of the substance into incineration plants  
 $F_{inc,others}^{in}$  is the inflow of the substance into incineration plants from sources other than the discarded products.  
 $F_{inc,t}^{out}$  is the total outflow of the substance from incineration plants.  
 $F_{inc,B}^{out}$  is the outflow of the substance from incineration plants in bottom ash.  
 $F_{inc,F}^{out}$  is the outflow of the substance from incineration plants in fly ash.  
 $F_{inc,A}^{out}$  is the emissions of the substance from incineration plants.  
 $F_{land,t}^{in}$  is the total inflow of the substance into landfill sites from all sources.  
 $F_{land,others}^{in}$  is the inflow of the substance into landfill sites from sources other than the discarded products.  
 $F_{land,t}^{out}$  is the total outflow from landfill sites.  
 $F_{ST}^{in}$  is the inflow of the substance into sewage treatment plants.  
 $F_{C,E,ST}^{out}$  is the flow of the substance originating from the emissions during the use phase.  
 $F_{pp,E}^{out}$  is the flow of the substance originating from the production processes.  
 $F_{C,FA,ST}^{out}$  is the flow of the substance originating from the consumption of food and animal products.  
 $F_{ST,SS}^{out}$  is the outflow of the substance from sewage treatment processes in sewage sludge.  
 $F_{ST,W}^{out}$  is the outflow of the substance from sewage treatment processes in water.  
 $F_{SS,S}^{out}$  is the flow of the substance with sewage sludge applied to soil.  
 $F_{SS,INC}^{out}$  is the flow of the substance with incinerated sewage sludge.  
 $F_{SS,L}^{out}$  is the flow of the substance with landfilled sewage sludge.

$F_{S,Y}^{in}$  is the inflow of the substance through mixed primary resources.  
 $F_{S,x}^{out}$  is the outflow of the substance to a specific destination.  
 $F_S^{in}$  is the inflow of the substance into agricultural soil.  
 $F_{AD,S}^{out}$  is the deposited flow from air into agricultural soil.  
 $F_{F,S}^{in}$  is the flow of the substance through fertilizers into agricultural soil.  
 $F_{M,S}^{in}$  is flow of the substance through manure into agricultural soil.  
 $F_{S,FOOD}^{out}$  is the uptake outflow of the substance from agricultural soil to food  
 $F_{S,FODDER}^{out}$  is the uptake outflow of the substance from agricultural soil to fodder  
 $F_{S,L}^{out}$  is the leaching outflow of the substance from agricultural soil to water.  
 $F_{An}^{in}$  is the inflow of the substance into animal production.  
 $F_{An}^{out}$  is the outflow of the substance from animal production.  
 $F_{CFA,An}^{in}$  is the inflow of the substance into the consumption of food and animal products from animal production.  
 $F_{CFA}^{in}$  is the total inflow of the substance into the consumption of food and animal products.  
 $F_{CFA}^{out}$  is the total outflow of the substance from the consumption of food and animal products.  
 $F_{CFA,ST}^{out}$  is the outflow of the substance from the consumption of food and animal products to sewage treatment.  
 $F_{PP,IA}^{out}$  is emissions from the production of different applications.  
 $F_{inc,A}^{out}$  is emissions from the incineration process.  
 $F_{R,A}^{out}$  is emissions from the recycling processes.  
 $F_{C,E}^{out}$  is emissions from the use of different applications.  
 $F_{NIU,A}^{out}$  is emissions from non-intentional use.  
 $F_A^{out}$  is the total outflow of the substance from air.  
 $F_{A,DS}^{out}$  is the deposited flow of the substance in soil.  
 $F_{A,DW}^{out}$  is the deposited flow of the substance in water.  
 $F_{A,TF}^{out}$  is the deposited flow of the substance outside the modelled system.  
 $F_{PP,i,W}^{out}$  is emissions from the production of different applications.  
 $F_{R,W}^{out}$  is emissions from the recycling processes to water.  
 $F_{NIU,W}^{out}$  is emissions from non-intentional use to water.  
 $F_{A,DW}^{out}$  is the deposition from air to water.  
 $F_{land,W}^{out}$  is the leaching from landfill sites to water.  
 $F_{ST,W}^{out}$  is the effluent from sewage to water.  
 $F_S^{in}$  is the inflow into the stock in non-agricultural soil.  
 $F_S^{out}$  is the outflow from the stock in non-agricultural soil.  
 $F_{C,E}^{out}$  is emissions from the use of different applications to non-agricultural soil.  
 $F_{NIU,A}^{out}$  is emissions from non-intentional use to non-agricultural soil.  
 $F_{A,DS}^{out}$  is the deposition from air to non-agricultural soil.  
 $F_{land,S}^{out}$  is the leaching from landfill sites to non-agricultural soil.  
 $F_{Res}^{in}$  is the addition to the stock of resources.  
 $F_{Res}^{out}$  is the outflow of the substance from the stock of resources.  
 $F_P^{in}$  is the inflow of the substance to its primary production processes.

## **Appendix B 2 – List of symbols in chapter 6**

**AEEPC** is air emissions from electricity production from coal  
**AEEPO** is air emissions from electricity production from oil  
**AEIN** is air emissions from incineration plants  
**AEOHM** is air emissions from other heavy metals production  
**AEOP** is air emissions from oil production  
**BAC** is bottom ash from coal fired power plants  
**BAIN** is bottom ash from incineration  
**FAC** is fly ash from coal fired power plants  
**FAIN** is fly ash from incineration  
**LOHM** is the landfilled stream from the production of other heavy metals  
**LSM** is the landfilled stream of secondary materials (fly ash and bottom ash)  
**LSS** is the landfilled stream of sewage sludge  
**MPR** is mixed primary resources  
**RZP** is refined zinc production  
**SEOP** is soil emissions from oil production  
**SPIS** is iron and steel slag  
**SS** is sewage sludge  
**WEOHM** is water emissions from other heavy metals production  
**WEOP** is water emissions from oil production  
**WEST** is water emissions from sewage treatment plants  
**WSIA** is waste stream from intentional applications  
**WWOHM** is waste water from other heavy metals production

## **Appendix B 3 – List of symbols in chapter 7**

**BAC** is coal fired power plants bottom ash  
**BAIN** is incineration bottom ash  
**FAC** is coal fired power plants fly ash  
**FACAG** is coal fired power plants fly ash applied in aggregates  
**FACAS** is coal fired power plants fly ash applied in asphalt  
**FACB** is coal fired power plants fly ash applied in building materials  
**FAIN** is incineration fly ash  
**LFAIN** is landfilled fly ash from the incineration plants  
**OHM** is other heavy metals  
**SPIS** is iron and steel slag  
**SS** is sewage sludge  
**UFAIN** is utilized fly ash from the incineration plants



## Publications in this thesis

Chapter	Reference
4	Elshkaki, A., Voet, E. van der, Holderbeke, M. van, and Timmermans, V. Dynamic Stock modelling: A method for the identification and estimation of future waste streams and emissions based on past production and product stock characteristics. <i>Energy</i> 2005; 30, 8, 1353-1363.
5	Elshkaki, A., Voet, E. van der, Holderbeke, M. van, and Timmermans, V. The environmental and economic consequences of the developments of lead stocks in the Dutch economic system. <i>Resources, Conservation and Recycling</i> 2004; 42: 133-154.
6	Elshkaki, A., Voet, E. van der, Holderbeke, M. Van, Timmermans, V. Long term consequences of non-intentional flows of substances: Modeling non-intentional flows of lead in the Dutch economic system and evaluating their environmental consequences. (submitted).
7	Elshkaki, A. and Voet, E. van der. Holderbeke, M. Van, Timmermans, V. Long term consequences of non-intentional flows of substances: Long-term consequences of substances presence in utilized secondary materials. (submitted).
8	Elshkaki, A., Voet, E. van der. The consequences of the use of platinum in new technologies on its availability and on other metal cycles. In Loeffe, C. V., (Editor). <i>Conservation and Recycling of Resources: New Research</i> . Nova Science Publisher, ISBN 1-60021-125-9. 2006.



## Summary

The research presented in this thesis is aimed at developing a dynamic substance flow-stock model that can be used to estimate future resource availability, emissions and waste streams. The research follows three consecutive stages:

- The first part develops a dynamic stock model, which combines elements from both physical and economic models, and establishes a link to a flow model, thus creating a dynamic substance flow-stock model.
- The second part develops a software tool able to carry out the dynamic substance flow-stock model.
- The third part implements the model in two case studies relevant to environmental policy. The first case study investigates the environmental and economic consequences of the development of lead stocks in the EU and the Netherlands. The second case study investigates the potential impacts of using platinum in the newly introduced fuel cell technology and addresses issues of both resource availability and environmental impacts.

This thesis consists of 9 chapters. Chapter 1 provides the introduction. Chapters 2 and 3 are dedicated to methodological aspects in substance flow analysis (SFA) and a representation of the dynamic substance flow-stock model. Chapters 4 to 8 include applications of the model in case studies. Chapter 9 is dedicated to a general discussion, conclusions and recommendations of aspects related to the substance flow-stock model and its applications.

## Methodology

In chapter 3, the dynamic substance flow-stock model is presented. The first sections of each of the consecutive chapters (chapters 4 to 8) discuss methodological aspects specifically related to the case studies.

## General

The model developed and presented in this thesis extends the currently available SFA models in three respects. Firstly, by combining flows and stocks. Secondly, it combines physical and economic elements. And thirdly, it operates at two levels: those of products and substances.

The model includes two subsystems; the economic and the environmental. The economic subsystem includes four processes, (extraction, production, consumption and waste management), several flows and several stocks. The main stocks in the economic subsystem are the stock of the substance in use, the stock of the substance in agricultural soil and the stock of the substance in landfill sites. Although agricultural soil may be regarded as an environmental compartment, it is treated in the model as part of the economic subsystem. Landfill sites are also treated as part of the economic subsystem. The environmental compartments in the model are limited to the air, water and non-agricultural soil. The model treats these environmental compartments as sinks. The environmental flows and stocks that arise as a consequence of economic activities that use the substance are specified in detail. Transboundary environmental flows, in and out of the system are assumed to be equal when the model is applied to national or local systems. It is not necessary to make this assumption when the model is applied at a global level. The main stocks in the environmental subsystems are the stock of the substance in the biosphere and the stock of the substance in non-agricultural soil.

The model uses two approaches to model the stock-in-use, and the flows of substances into (the inflow) and out of (the outflow) the stock-in-use. The first approach starts by taking historical data on the inflow and the product lifetime. The second approach starts by taking historical data on the stock-in-use, the inflow, and the product lifetime. Two approaches are used to model the inflow of substances into the stock-in-use. In the first, the inflow of substances is modelled based on two equations; one describing the inflow of products and the other describing the substance content of products. Each one is determined by different

factors. For each product, the inflow into the stock-in-use is modelled based on a regression model that describes the inflow as a function of selected socio-economic variables. The socio-economic variables used in the model are GDP, per capita GDP, sectoral share of GDP, population, and material price. A time variable is used as a proxy of the influence of other variables. Some of the variables in the model are exogenous (GDP and population) and others are endogenous (price). The substance content of products is treated either as constant or changing overtime. It is modelled either as a function of time or by using the learning curve concept. The learning curve concept, which introduces endogenous technical change into the dynamic model, is adapted to model the substance content as a function of the cumulative production. In the second approach, the inflow of the substance into the stock-in-use is modelled directly by one equation using different types of models (linear model, log-log model and the intensity-of-use technique). This approach is used when the data on the substance level (the total amount of the substance used in certain products) is directly available. In this case, the explanatory variables used in the model cover both the product inflow and substance content. Although the first approach has several advantages, sometimes the second approach is necessary as, most data sources directly provide the consumption of substances. The outflow is based mainly on the physical mechanisms of leaching and delay. The leaching model estimates the outflow out of the stock-in-use due to emissions during use, through corrosion, evaporation and suchlike, expressing this as a fraction of the stock-in-use. The emission factors may change over time and are determined by a wide range of factors, such as the surrounding atmosphere, the weather, maintenance, and others. The delay model estimates the discarded outflow as a delayed inflow with a certain life span. The product life span is never exactly known, however it can take an average value or be assumed to fit a Weibull distribution based on available information. Other distributions are possible. In extreme situations - for example a very long life span, or a very wide, narrow or skewed distribution - this may considerably influence the results.

The geological stock of a substance is treated as the economic stock. The model takes the geological stock of substances as including the currently known reserve and identified resources. Depending on the initial stock in the model, additions (inflows) to the resource stock can include newly found ores, or existing ores that become profitable. The extracted flow (the outflow from the resource stock) is mainly determined by the demand for the substance and the availability of secondary materials. The mechanisms through which the impacts of price increases and the development of new technologies may influence a possible increase in the resource stock (by making the currently known resource stock more profitable or low-grade resources possible to be extracted) are not included in the model. These known resources are already included in the identified resources. The possibility of finding new ores, which might increase the availability of resources, is not included in the model.

The stock of the substance stock in landfill sites is determined by the inflow of the substance into landfill sites and the leaching outflow from them. The inflow of the substance to landfill sites originates from different parts of the economic subsystem and the leaching outflow is determined by the substance characteristics and landfill technology.

The stock of the substance in agricultural soil is mainly determined by flows into and out of agricultural soil. Flows into agricultural soil are mainly from atmospheric deposition, the use of fertilizers, and the use of sewage sludge and manure. The outflow is mainly determined by the uptake rate of food and fodder.

As with substance flow analysis, the substance flow-stock model can be applied at different levels: international, national, and local. If the modelled system is small (national or local), disconnections will exist between the different compartments of the economic subsystem (extraction, production, consumption, and waste management) as a result of trade (the import and export of the refined substance, of products containing the substance and of obsolete products.). The smaller the country, the stronger this disconnection will be. This disconnection does not exist when the model is applied at the global level. The dynamic substance flow-stock model presented in this thesis treats the import and export of products, obsolete products and refined substances as a net import, which is estimated as a balancing item.

### ***Lead case study***

The model includes flows and stocks of lead in the economic subsystem and the environmental flows and stocks that are directly linked to economic activities. The model includes the most significant intentional applications of lead, such as batteries, lead sheet, cathode ray tubes and cable sheathing. It also includes non-intentional applications of lead, such as the utilization of secondary flows (fly and bottom ash) in road construction material, building materials and agricultural soil. These applications are assumed to be sufficient to estimate the waste streams and emissions of lead. Transboundary flows of lead and other flows and stocks that result from the loops and cycles within the environmental subsystem itself are not been treated in detail.

In modelling the inflow, outflow and stock of lead in use for lead applications, the first approach, that starts from the historical data on the inflow and the products' life span is adopted. The one exception to this is that of cathode ray tubes, for which the flows and stocks are modelled based on the second approach. The inflow of lead into the stock-in-use of its different applications is modelled based on the substance/product approach, with the explanatory variables (GDP, per head GDP, population, and time) being exogenously determined. These variables appeared to be sufficiently explaining a number of past trends of these flows, such as the inflow of lead to the consumption phase, the production of refined lead, the production of other heavy metals and the production of oil and its use in electricity production. However they appeared insufficient in describing the past trend of the inflow of phosphate fertilizers and the production of electricity from coal. Therefore, in modelling these flows time is used as a proxy of the effect of other influential variables. In the case of fertilizers, other explanatory variables, such as the number of animals and the agricultural yield could also have been used in the analysis. However, these variables have not been used in the Dutch case, as it is clear that the most influential variables are related to policy. Therefore, the future use of fertilizer is estimated using time as the explanatory variable as this captures the impact of policy. A minimum value on the use of fertilizers is set in the model based on a scenario developed by RIVM. The past use of coal for electricity production could not be directly explained by the explanatory variables, but they were sufficient to describe total electricity production and production of electricity from other sources. Therefore, it was possible to estimate the production of electricity from coal as a balancing variable. The discarded outflow of lead applications is modelled using data on past inflows and specific life spans, which are assumed to fit a Weibull distribution.

Imports and exports at different stages in the economic subsystem are treated as a net import which is estimated as a balancing item of the two different compartments.

Different assumptions are used regarding the initial stocks of different stock-building applications of lead in the consumption phase and the stocks of lead in landfill sites. The initial stock-in-use of different lead applications are estimated based on the availability of these applications in a specific year, which is used as the starting point for the calculations. These stocks will not affect the outcome of the model if the difference between the starting year of the past inflow and the starting year of the future calculation is greater than the application's life span. The initial stock of lead in landfill sites is difficult to find. The model assumes the initial stock of lead in landfill sites to be zero. This assumption will affect estimates of the future stock and of the outflow of lead from landfill sites, both of which will be underestimated.

### ***Platinum case study***

The model focuses mainly on the economic subsystem and includes the extraction and production of Pt (from both primary and secondary resources), and the production, consumption and waste management of applications containing Pt. These include fuel cells, catalytic converters, and other uses in the chemical, electrical and electronic, glass and petroleum industries, investment, jewellery and other applications. The model also includes the production of co-produced metals (Ni and Cu) from Pt primary resources, the consumption and waste management of Ni and Cu applications and the production of Ni and Cu from secondary resources. The model includes emissions to the environment and the resource stock in the environment.

The demand for Pt is looked at globally and supply comes from four sources (The Republic of South Africa, Russia, the USA and Canada, and other countries). Pt ores are identified as Platinum Group Elements (PGE) dominant ores, Ni-Cu dominant ores and miscellaneous ores, depending on the geographical distribution. Pt resources in these ores are classified as current reserve and identified resources.

The model consists of a set of differential equations describing the change of the magnitude of the stock of Pt in the system's compartments over time. There is assumed to be no change in the magnitude of the economic stock of the substance over time in relation to the production processes, the collection processes, and the recycling processes of Pt applications, and in the Pt market (i.e. the input is equal to the output). The changes of the magnitude of the stock of Pt in use and the resource stock of Pt over time are determined by the inputs into and the outputs from these stocks. In addition,, the model consists of several model relations describing the inflow of substances into the stock-in-use as functions of the socio-economic variables.

The inflow and outflow of Pt and the stock of Pt in use in all Pt applications are modelled based on the first approach that starts from historical data on the inflow and the products' life spans. The main driving force in the model is the global demand for Pt. This is estimated from the demand for its applications (Fuel Cells (FC), Catalytic Converters (CC), and other applications) and the amount of Pt required for each application. The inflow of Pt into the stock-in-use of FC and CC is modelled using the substance/product approach. The inflow of Pt into the stock-in-use of other applications is modelled using the substance approach. The demand for Pt applications is modelled based on socio-economic variables such GDP, per capita GDP, population size, and material price. Some of the explanatory variables, such as GDP and population, are exogenously determined and others, such as the price and technological development, are endogenously determined. Different scenarios for FC market penetration are used to estimate the demand for FC and the replacement of CC. The Pt required for each application is modelled as a function of accumulated production using the learning curve. Scenarios used for the market penetration of FC and the progress ratios used in the learning curve have a great impact on the model outcome. Several other factors are important in determining the model outcome. These include the life span of the applications, the collection rates of the discarded applications and the efficiency of production processes (primary and secondary). The discarded outflow of Pt applications is modelled from the past inflow and a specific life span, which is taken as an average value.

The initial stock in the use phase is assumed to be zero. This assumption will not have any impact on the model outcome in terms of resource availability. However, it will lead to an underestimation of the magnitude of the stock in the use phase. The initial resource stock in the biosphere has been given two values. The first is the value of the current reserve and the second is the value of identified resources.

An analysis is carried out to examine the sensitivity of the model outcome to the parameters in the model.

## Case studies

### *Lead*

The first case study, of lead, is presented in chapters 4 to 7. These chapters describe the modelling aspects, present the data, and analyse the long-term management of the intentional and non-intentional use of lead. The lead case study is mainly aimed at:

- evaluating the economic and environmental consequences of the developments of lead stocks on the long-term management of lead;
- evaluating the long-term direct environmental consequences of non-intentional flows of lead and compare them to those of its intentional flows and;
- evaluating the long-term environmental and economic consequences of non-intentional existence of lead in applications.

The main outcome of the model suggests that in the Netherlands the amount of lead available for recycling is expected to exceed the demand for lead in the near future. This model however, is restricted to one country and more general conclusion about lead availability and demand would require an analysis on a larger scale (regional or global) where imports and exports would play a lesser role. If comparable developments can be detected on a larger scale as well, this finding may have consequences for the future management of lead. It would suggest that the demand for lead is dropping as a result of policies designed to phase out its use. On the other hand, the supply from secondary sources is increasing as a result of the past build up of stocks in society. Moreover, the supply from primary sources continues and is expected to continue for reasons other than meeting new demand for lead. All this may have consequences for the price of lead, for the profitability of primary production and the recycling industry. As a result the landfill and incineration streams might increase at the expense of recycling, and ultimately may lead to an increase in emissions. The model also suggests that the environmental consequences of the non-intentional use of lead from zinc and iron ores and from coal are more severe than those originating from the waste streams of the intentional applications of lead. The amount of lead generated by non-intentional sources is sufficient to provide at least part of the total demand for lead. Therefore, special attention should be given to managing these non-intentional flows of lead, especially those originating from mixed primary resources containing lead as a contaminant (zinc and iron ores and coal). In addition, recovery of the available lead in secondary materials, such as fly and bottom ashes generated from coal fired power plants and waste incineration plants prior to landfilling or use as construction materials is recommended. The residues of production and consumption of non-intentional applications of lead can be seen as potential sources for lead, and other metals, in the future.

### ***Platinum***

The second case study is presented in chapter 8 and concerns the use of platinum in the newly introduced fuel cell technology. This case study aims at:

- investigating the potential long-term impact of the increased use of platinum in fuel cell technology and other applications in terms of future resource availability and;
- evaluating the long-term consequences of the increased demand for platinum on the cycles of other co-produced metals, especially Ni and Cu

The model shows that the main losses of platinum occur in the waste management of fuel cells and catalytic converters and the production of platinum from primary sources. The main outcome of the model suggests that current reserves and identified resources of platinum will be depleted before the end of the century if no additional measures are taken. However, the model also suggests that there some factors on the demand and supply sides may extend the availability of platinum over time. These include: the increasing efficiency of fuel cell production, the market penetration of fuel cells, together with the increasing efficiency of the waste management of fuel cells and catalytic converters, the increasing efficiency of the production of platinum from primary sources, and the increasing life span of fuel cells. Technological developments in fuel cell production can play an important role in increasing the availability of platinum, as can improvements in mining technologies. Moreover, it is recommended that fuel cell technology be gradually introduced to the market and to investigate the possibility of finding other sources of supply of platinum. Platinum has been accumulating in the soil since the introduction of catalytic converters and this could represent a potential source of platinum in the future. Other sources include mixed primary resources.

The model also shows that the metals co-produced with platinum (Cu and Ni) will be affected by the increased production of platinum. The possibility of an oversupply of these co-produced materials might have consequences in terms of their secondary production and their primary production from other sources. The outcome of the model suggests this will not have major consequences that for the copper cycle as the demand for copper is very high compared to the supply from this source. For nickel, the story is different as the supply of this metal from platinum ores is expected to exceed its demand, which will have profound consequences for both the primary mining and the recycling of nickel.

## **General discussion, conclusions and recommendations**

Chapter 9 provides a general discussion, with conclusions and recommendations of aspects related to the substance flow-stock model and its application in the case studies.

In the first part of chapter 9, a number of issues related to the dynamic flow-stock model are discussed. These mostly pertain aspects relating to the combination of flows and stocks, the combination of physical and economic elements, the level of scale in modelling substance flow and stocks, the inclusion of the economic and environmental subsystems, operating at the levels of products and substances and the role of uncertainty. It is recommended that a substance flow-stock model should include both economic and physical-chemical variables as substance flows through the economy are basically determined by the economic demand for substance-containing applications. In turn, substance flows out of the economy in the shape of waste and emissions are primarily determined by the physical-chemical properties of the substance. It is also recommended to include different factors or explanatory variables that cover different economic driving forces: the demand for products containing the substance, the demand for secondary materials and policies on waste. It also recommends using the product/substance approach and learning curve concept to model the flow of substances into the stock-in-use and the substance content of products.

## **Recommendations for further development**

Some interesting subjects for future research in the area of dynamic substance flow analysis are: the inclusion of trade in national dynamic substance flow-stock models, the inclusion of the mechanisms describing the impacts of price and technology development on the resource stock in the biosphere and the inclusion of the impacts of energy use in the mining processes in global dynamic substance flow-stock models. Worthwhile opportunities also exist to investigate the possibilities of linking the dynamic substance flow-stock model to other environmental models, such as environmental fate models and environmental risk assessment models. This could improve estimates of the environmental concentration of substances in environmental media and enhance assessment of the risks entailed.



## Samenvatting

Het onderzoek dat in deze thesis wordt gepresenteerd is gericht op de ontwikkeling van een dynamisch stof-stroom-voorraadmodel dat kan worden gebruikt om de toekomstige beschikbaarheid, uitstoot en afvalstromen te schatten. Het onderzoek heeft in drie opeenvolgende fasen plaatsgevonden:

- In de eerste fase werd een dynamisch voorraadmodel ontwikkeld dat elementen combineerde van fysieke en economische modellen; hierbij werd een relatie gelegd naar een stroommodel. Hierdoor kwam een dynamisch stof-stroom-voorraadmodel tot stand.
- In de tweede fase werd een software programma ontwikkeld waarmee het dynamisch stof-stroom-voorraadmodel uitgevoerd kon worden.
- In de derde fase werden twee casus studies, relevant voor milieubeleid, ingevoerd in het softwareprogramma. In de eerste casus werden de gevolgen voor economie en milieu onderzocht van de loodvoorraden in de EU en Nederland. In de tweede casus werd onderzoek gedaan naar de mogelijke gevolgen van het gebruik van platina in de onlangs geïntroduceerde brandstofceltechnologie. Ook werden de beschikbaarheid van de grondstof en het milieueffect onderzocht.

Deze thesis bestaat uit negen hoofdstukken. Hoofdstuk 1 bevat de introductie, hoofdstukken 2 en 3 zijn gewijd aan de methodologische aspecten van stof-stroomanalyse (Engels acroniem: SFA) en aan een weergave van het dynamische stof-stroom-voorraadmodel. Hoofdstukken 4 t/m 8 bevatten toepassingen van het model in casus studies. In hoofdstuk 9 worden een algemene discussie, conclusies en aanbevelingen betreffende aan het stof-stroom-voorraadmodel gerelateerde aspecten en de toepassingen daarvan gepresenteerd.

## Methodologie

In hoofdstuk 3 wordt het dynamische stof-stroom-voorraadmodel gepresenteerd. In de eerste delen van elk van de volgende hoofdstukken (4-8) worden methodologische aspecten besproken die aan de casus studies zijn gerelateerd.

## Algemeen

Het ontwikkelde en hier gepresenteerde model gaat in drie opzichten verder dan de huidige beschikbare SFA-modellen. In de eerste plaats door de combinatie van stromen en voorraden, ten tweede door de combinatie van fysieke en economische elementen en op de derde plaats opereert het model op twee niveaus: stoffen en producten.

Het model omvat twee subsystemen: het economische en het milieu. Het economische subsysteem omvat vier processen (delving, productie, consumptie en afvalbeheer), diverse stromen en diverse voorraden. De belangrijkste voorraden in het economische subsysteem zijn de voorraad “stof-in-gebruik”, de voorraad stof in landbouwgrond en de voorraad stof op afvalverwerkingslocaties. De milieuaspecten van het model zijn beperkt tot lucht, water en niet-agrarische grond. Het model ziet deze onderdelen als verzamelplaatsen. De belangrijkste voorraden in de milieugebonden subsystemen zijn de voorraden stof in de biosfeer en de hoeveelheid stof in niet-agrarische grond.

In het model worden twee benaderingen gebruikt om de voorraad-in-gebruik en de stofstromen naar (instroom) en uit (uitstroom) de voorraad-in-gebruik weer te geven. De eerste benadering verzamelt historische gegevens betreffende de instroom en levensduur van het product. De tweede benadering verzamelt historische gegevens betreffende voorraad-in-gebruik, de instroom en de levensduur van het product. De twee benaderingen worden gebruikt om de instroom van materialen in de voorraad-in-gebruik weer te geven. In de eerste benadering wordt de instroom van materie weergegeven op basis van twee vergelijkingen: een om de instroom van producten te beschrijven en de ander om de hoeveelheid stof in producten te beschrijven. Elk wordt door verschillende factoren bepaald. In de tweede benadering wordt de

instroom van het stof in de voorraad-in-gebruik direct weergegeven door een vergelijking waarbij verschillende modellen worden gebruikt (lineair model, log-log model, en gebruiksintensiteit-techniek). Deze aanpak wordt gebruikt wanneer de gegevens over stofgehalte (de totale hoeveelheid stof gebruikt in bepaalde producten) direct beschikbaar zijn. De uitstroom is hoofdzakelijk gebaseerd op de fysieke mechanieken van uitloggen en vertraging. In het loogmodel wordt een schatting gemaakt van de uitstroom uit de voorraad-in-gebruik als gevolg van uitstoot gedurende gebruik door onder andere corrosie en verdamping en dergelijke. Dit wordt uitgedrukt als een deel van de voorraad-in-gebruik. In het vertragingmodel wordt een schatting gemaakt van de afgedankte uitstroom als een vertraagde instroom met een bepaalde levensduur.

De geologische voorraad van een stof wordt gezien als de economische voorraad. Deze voorraden bestaan uit de op dit moment bekende reserves en vastgestelde bronnen. Afhankelijk van de voorraad waar in het model mee wordt begonnen, kunnen toevoegingen (instroom) aan de bestaande voorraad uitsluitend bestaan uit nieuw gevonden vindplaatsen of bestaande vindplaatsen die winstgevend worden. De onttrokken stroom (de uitstroom uit de bronvoorraad) wordt hoofdzakelijk bepaald door de vraag naar het stof en de beschikbaarheid van secundair materiaal. In het model zijn niet opgenomen de mechanismen waardoor de invloed van prijsstijgingen en de ontwikkeling van nieuwe technologieën een stijging van de bronvoorraad kunnen beïnvloeden (door de nu bekende bronvoorraad rendabeler te maken of laag gewaardeerde bronnen mogelijkserwijs te gebruiken). Deze bekende bronnen zijn al opgenomen in de vastgestelde bronnen. De mogelijke ontdekking van nieuwe vindplaatsen waardoor de beschikbaarheid van grondstoffen wordt vergroot, wordt niet in dit model opgenomen.

De voorraad in afvallocaties wordt bepaald door de instroom van het stof in de afvallocaties en de uitlopende uitstroom daarvan. De instroom van het stof in afvallocaties is afkomstig uit verschillende delen van het economische subsysteem en de uitlog uitstroom wordt bepaald door de stoffeigenschaften en de technologie van de afvalverwerkende locatie. De voorraad stof in agrarische grond wordt met name bepaald door stromen in en uit de agrarische grond. Bij instromen kan men denken aan neerslag, kunstmest, gier of mest. De uitstroom wordt voornamelijk bepaald door het opnemende vermogen van wat er op het land wordt verbouwd.

### ***Lood casus studie***

Dit model omvat stromen en voorraden lood in het economische subsysteem en de milieustromen en voorraden die direct gerelateerd zijn aan economische activiteiten. Het model bevat de meest belangrijke intentionele toepassingen van lood, zoals batterijen, loodplaten, kathodestraalbuizen en kabelomhulsels. Het omvat ook niet-intentionele toepassingen van lood, zoals het gebruik van secundaire stromen (vlieg- en bodemas) in wegomateriaal, bouwmateriaal en agrarische grond. Er wordt aangenomen dat deze toepassingen voldoende zijn om een raming te kunnen maken van de afvalstromen en uitstoot van lood.

Bij het modelleren van de in- en uitstroom en loodvoorraad-in-gebruik voor toepassingen van lood, wordt de eerste benadering, die uitgaat van de historische gegevens betreffende de instroom en levensduur van het product, gebruikt. Uitzondering hierop vormt de kathodestraalbuis, hiervoor worden stromen en voorraden in het model ingevoerd op basis van de tweede benadering. Het model waarin de instroom van lood in de voorraad-in-gebruik van de verschillende toepassingen wordt ingevoerd, is gebaseerd op de benadering stof/product, met de verklarende variabelen (BNP, per hoofd BNP, bevolking en tijd) exogeen bepaald. Deze variabelen leken een aantal trends in het verleden van deze stromen voldoende te beschrijven, zoals de loodinstroom naar de verbruikersfase, de productie van gezuiverd lood, de productie van andere zware metalen en de olieproductie en het gebruik in de elektriciteitsproductie. Ze leken echter de historische trend van de instroom van fosfaathoudende kunstmest en de productie van elektriciteit uit kolen onvoldoende te beschrijven. Daarom is bij het opstellen van deze modellen tijd gebruikt als een vervanger van het effect van overige beïnvloedbare variabelen.

De afgedankte uitstroom van loodtoepassingen wordt in het model ingebracht waarbij historische gegevens worden gebruikt betreffende instroom en specifieke levensduur in het verleden. Hierbij wordt aangenomen dat deze passen in een Weibull-distributie.

De aanvankelijke voorraad-in-gebruik van verschillende loodtoepassingen wordt geschat op de beschikbaarheid van deze toepassingen in een bepaald jaar, hetgeen wordt gebruikt als startpunt voor de

berekeningen. De aanvangshoeveelheid van de loodvoorraad in afvallocaties is moeilijk te vinden. Het model gaat er vanuit dat de aanvankelijke loodvoorraad in afvallocaties nul bedraagt.

### ***Platina casus studie***

Het model richt zich hoofdzakelijk op het economische subsysteem en bevat de delving en productie van platina (zowel uit primaire als secundaire bronnen) en de productie, verbruik en afvalbeheersing van toepassingen die platina bevatten. Hiertoe behoren onder andere brandstofcellen, katalysators en andere toepassingen in de chemische, elektrische en elektronische industrie, glas- en olie-industrie, investeringen, juwelen en andere toepassingen. Het model omvat ook de productie van gelijktijdig geproduceerde metalen (Ni en Cu) uit primaire platinabronnen, het verbruik en de afvalbeheersing van Ni en Cu toepassingen en de productie van Ni en Cu uit secundaire bronnen. Het model omvat emissies in het milieu en de bronvoorraad in het milieu. De vraag naar platina wordt mondiaal bekeken en aanvoer komt uit vier bronnen (Zuid-Afrika, Rusland, VS en Canada, en andere landen).

Het model bestaat uit een set differentiaalvergelijkingen die de verandering van de grootte van de voorraad platina in de tijd beschrijven in de compartimenten van het systeem. De in- en uitstroom van platina en de voorraad platina-in-gebruik in alle platina toepassingen zijn in het model ingebracht gebaseerd op de eerste benadering, die uitgaat van historische gegevens betreffende de invoer en levensduur van de producten. De belangrijkste drijvende kracht in het model is de mondiale vraag naar platina. Dit wordt geschat op basis van de vraag naar de toepassingen (Fuel Cells, ofwel FC's (brandstofcellen), katalysators (Engels acroniem CC) en andere toepassingen) en de benodigde hoeveelheid platina voor iedere toepassing. De instroom van platina in de voorraad-in-gebruik van FC en CC wordt in het model ingebracht met gebruik van de stof/product benadering. De instroom van platina in de voorraad-in-gebruik van andere toepassingen wordt in het model opgenomen met gebruik van de stofbenadering. Sommige verklarende variabelen, zoals het BNP en bevolking, worden exogeen bepaald en andere, zoals prijs en technologische ontwikkelingen, worden endogeen bepaald. Verschillende scenario's voor FC marktpenetratie worden gebruikt om een raming van de vraag naar FC en de vervanging van CC te bepalen. De voor iedere toepassing benodigde platina wordt gemodelleerd als functie van een geaccumuleerde productie met gebruikmaking van de leercurve. De afgewerkte uitstroom van platinatoepassingen wordt gemodelleerd op basis van instroom in het verleden en een specifieke levensduur, welke als een gemiddelde waarde wordt aangenomen. De aanvangsvoorraad in de gebruiksfase wordt aangenomen op nul. Deze aanname heeft geen invloed op de uitkomst van het model wat betreft beschikbaarheid van bronnen. Aan de bronvoorraad bij aanvang in de biosfeer worden twee waarden gegeven. De eerste is de waarde van de huidige reserve en de tweede is de waarde van de vastgestelde bronnen.

### **Casus studie**

#### ***Lood***

De eerste casus studie, waarbij lood wordt gebruikt, wordt gepresenteerd in hoofdstukken 4 t/m 7. Hierin worden de aspecten van de modellen beschreven, de gegevens gepresenteerd en vindt een analyse plaats van het intentionele en niet-intentionele gebruik van lood op lange termijn. De lood casus studie is voornamelijk gericht op:

- Evaluatie van de gevolgen voor economie en milieu van de ontwikkelingen van loodvoorraden op het beheer van lood op lange termijn;
- Evaluatie van de directe gevolgen voor milieu op lange termijn van niet-intentionele loodstromen en een vergelijking van deze met de intentionele stromen; en
- Evaluatie van de gevolgen op lange termijn voor milieu en economie van niet-intentionele aanwezigheid van lood in toepassingen.

De belangrijkste uitkomst van het model suggereert dat in Nederland de hoeveelheid voor recycling beschikbaar lood naar verwachting de vraag naar lood in de nabije toekomst overschrijdt. Dit model is echter beperkt tot één land; een meer algemene conclusie wat betreft de hoeveelheid beschikbaar lood en de

vraag naar lood verlangt een analyse op grotere schaal (regionaal of mondiaal), waarbij im- en export een ondergeschikte rol spelen. Als ook op grotere schaal vergelijkbare ontwikkelingen worden ontdekt, kunnen de bevindingen gevolgen hebben voor het toekomstige beheer van lood. Het zou kunnen suggereren dat de vraag naar lood afneemt als gevolg van beleid om het gebruik uit te bannen. Aan de andere kant groeit de toelevering uit secundaire bronnen als gevolg van de voorraden die in het verleden in de maatschappij zijn opgebouwd. Bovendien houdt de toevoer uit primaire bronnen aan en zal naar verwachting ook aanhouden om andere redenen dan nieuwe vraag naar lood. Dit alles kan gevolgen hebben voor de prijs van lood, de winstgevendheid van de primaire productie en de recyclingindustrie.

Als gevolg hiervan zouden de stromen naar afvalverwerking en verbranding kunnen stijgen ten koste van recycling en dit zou uiteindelijk kunnen leiden tot een verhoging van uitstoot. Uit het model komt ook de suggestie naar voren dat de milieugevolgen van het niet-intentionele gebruik van lood uit zink- en ijzererts en uit kolen ernstiger zijn dan die afkomstig uit afvalstromen van de intentionele toepassingen van lood. De hoeveelheid lood geproduceerd door niet-intentionele bronnen is voldoende om ten minste te voldoen aan een deel van de vraag naar lood. Daarom zou er in het bijzonder aandacht geschonken moeten worden aan de beheersing van deze niet-intentionele loodstromen, vooral wat betreft de loodstromen afkomstig uit gemengde primaire bronnen die lood bevatten als vervuilde stof (zink- en ijzererts en kolen). Voorts wordt aanbevolen om de beschikbare hoeveelheid lood in secundaire materialen, zoals vlieg- en bodemas afkomstig uit kolengestookte energiecentrales en afvalverbrandingsinstallaties te herwinnen voordat deze afvalstoffen naar de afvalverwerking gaan of als constructiemateriaal worden gebruikt.

Het residu van productie en verbruik van niet-intentionele loodtoepassingen kan in de toekomst worden gezien als potentiële bronnen voor lood en andere materialen.

### ***Platina***

De tweede casus wordt in hoofdstuk 8 gepresenteerd en betreft het gebruik van platina in de onlangs geïntroduceerde brandstofceltechnologie. Het doel van de studie is:

- Onderzoek naar de mogelijke invloed van het toegenomen platinagebruik in brandstofceltechnologie en andere toepassingen in termen van toekomstige beschikbaarheid van bronnen op lange termijn; en
- Evaluatie van gevolgen op lange termijn van de toegenomen vraag naar platina op de cycli van andere, gelijktijdig geproduceerde metalen, met name Ni en Cu.

In het model wordt aangetoond dat de belangrijkste verliezen van platina optreden in de afvalbeheersing van brandstofcellen en katalysatoren en in de productie van platina uit primaire bronnen. De belangrijkste uitkomst van het model suggereert dat de huidige reserves en vastgestelde platinabronnen uitgeput zullen zijn voor het einde van de eeuw, indien er geen aanvullende maatregelen worden getroffen. Echter, uit het model blijkt ook dat bepaalde factoren aan de vraag- en toevoerzijde de beschikbaarheid van platina in verloop van tijd kunnen verlengen. Hierbij kan worden gedacht aan de toenemende effectiviteit van brandstofcelproductie, de marktpenetratie van brandstofcellen, de toenemende effectiviteit van afvalbeheersing van brandstofcellen en katalysators, de toenemende effectiviteit in de platinaproductie uit primaire bronnen, en de toenemende levensduur van brandstofcellen. Daarnaast kunnen technologische ontwikkelingen in de brandstofcelproductie een belangrijke rol spelen bij het vergroten van de beschikbaarheid van platina, evenals verbeteringen in de mijnstechnologie. Voorts wordt aanbevolen de brandstofceltechnologie geleidelijk op de markt te introduceren en onderzoek te doen naar de mogelijkheden om andere bronnen van platina te vinden. Sinds de introductie van katalysators heeft platina zich kunnen ophopen in de grond en dit zou in de toekomst een potentiële platinabron kunnen zijn. Tot andere mogelijke bronnen behoren de gemengde primaire bronnen.

Dit model laat ook zien dat de metalen die tegelijkertijd met platina worden geproduceerd (Cu en Ni) worden beïnvloed door de toenemende productie van platina. De mogelijke overproductie van deze gelijktijdig geproduceerde materialen kan gevolgen hebben wat betreft de secundaire productie en hun primaire productie uit andere bronnen. De uitkomst van het model suggereert dat dit geen grote gevolgen heeft voor de kopercyclus, daar de vraag naar koper erg groot is in vergelijking met de levering uit deze bron. Voor nikkel is het verhaal anders: volgens de verwachting overtreft de productie van dit metaal uit

platina-erts de vraag, wat vergaande gevolgen zal hebben voor zowel de winning uit primaire bronnen als het recyclen van nikkel.

### **Algemene discussie, conclusies en aanbevelingen**

In hoofdstuk 9 wordt een algemene discussie gevoerd, met conclusies en aanbevelingen van aspecten die gerelateerd zijn aan het stof stroom-voorraadmodel en de toepassing daarvan in de casus studies.

In het eerste deel van hoofdstuk 9 worden een aantal problemen besproken die verband houden met het dynamische stroom-voorraadmodel. Dit heeft voornamelijk betrekking op de combinatie van stromen en voorraden, de combinatie van fysieke en economische elementen, het schaalniveau van het modelleren van stofstromen en –voorraden, het meetellen van de economische en milieugerelateerde subsystemen die opereren op product- en stofniveau en de rol van onzekerheid. Het wordt aanbevolen in een stof-stroom-voorraadmodel zowel economische als fysiek-chemische variabelen als stofstromen door de economie op te nemen, omdat stofstromen door de economie primair worden bepaald door de economische vraag naar toepassingen die het betreffende stof bevatten. De uitstroom van stof uit de economie in de vorm van afval en uitstoot wordt echter primair bepaald door de fysiek-chemische eigenschappen van het stof. Het wordt eveneens aanbevolen verschillende factoren of verklarende variabelen toe te voegen die verschillende economische drijvende krachten vertegenwoordigen: de vraag naar producten waarin het stof is verwerkt, de vraag naar secundaire materialen en afvalbeleid. Het wordt tevens aanbevolen de product/stof-benadering en het leercurve-concept te gebruiken om de stofstroom in de voorraad-in-gebruik en de hoeveelheid stof in producten te modelleren.

### **Aanbevelingen voor verdere ontwikkeling**

Enkele interessante onderwerpen voor toekomstig onderzoek op het gebied van dynamische stof-stroomanalyses zijn: het meerekenen van handel in nationale dynamische stof-stroom-voorraadmodellen, het meerekenen van mechanismen die de invloed van prijs en technologieontwikkeling op de bronvoorraad in de biosfeer beschrijven, en het meerekenen van de invloed van energiegebruik bij delvingsprocessen in mondiale dynamische stof-stroom-voorraadmodellen.

Het is ook waardevol om de mogelijkheden te onderzoeken om het dynamische stof-stroom-voorraadmodel te koppelen aan andere milieumodellen, zoals lotgeval modellen en milieurisicobeoordeling modellen waarin milieurisico's worden beoordeeld. Dit zou de ramingen wat betreft de milieuconcentratie van stoffen in milieucompartimenten en daarmee samenhangende risicobeoordeling kunnen verbeteren.



## Curriculum Vitae

### *Personal*

Name Ayman Elshkaki  
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### *Education*

B.Sc., Chemical Engineering, El-Fateh University, Tripoli, Libya, 1996.  
M.Sc., Environmental Chemistry, Leiden University, Leiden, The Netherlands, 2000.  
Ph.D., Environmental Science, Leiden University (2007, expected)

### *Employment record*

Chemical Engineer, Palestinian Energy Authority, Gaza Strip, 1997-1998  
Student Assistance, Centre of Environmental Science - Leiden University, Leiden, 2000  
Chemical Engineer, Palestinian Ministry of Environmental Affairs, Gaza Strip, 2001  
Research Assistant, Centre of Environmental Science - Leiden University, Leiden, 2001- present

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